```
C:\STNEXP4\QUERIES\096237
chain nodes :
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```
11 12
          14
               15
                   16
                      17
                          18
                              20
                                  21
                                      24
                                                 27
                                         25
                                             26
                                                     30
                                                         31
                                                             32
                                                                33
                                                                    34
   35 .45
           46
               47
                   48
                      56
                          57
                              58
                                  59
                                      60
                                         68
ring nodes :
               5
   1 2 3 4
                  6
                   7
ring/chain nodes :
   29 38
           49
chain bonds :
   1-18 2-11 3-17 4-14 5-24 6-12 7-16 8-15
                                                 20-21
                                                        20-25
   26-29
          30-31 30-68 31-32
                              32-33
                                     33-34
                                           34-35 35-38 45-46 46-47
   47-48 48-49 56-57 57-58
                              58-59
                                     59-60
                                           60-61
ring bonds :
   1-2 1-6
             2-3 3-4 3-9 4-5
                                5-8
                                     6-7 7-8
exact/norm bonds :
                  2-3
                             3-4 3-9 3-17
   1-2 1-6
             1-18
                       2-11
                                           4-5
                                                 4-14 5-8 5-24 6-7
   6-12 7-8 7-9 7-16 8-15 20-21 20-25 26-27 26-29 30-31 31-32
   32-33 33-34
                34-35
                      35-38 45-46 46-47 47-48 48-49 56-57 57-58
   58-59 59-60
                60-61
exact bonds :
   30-68
isolated ring systems :
   containing 1 :
```

G1:Ak,H

G2:H,[*1],[*2]

G3:C, N

G5:H, [*3], [*4], [*5]

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Match level :
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 29:CLASS 31:CLASS 32:CLASS 34:CLASS 35:CLASS 30:CLASS 33:CLASS 38:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 45:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 68:CLASS

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L13

(FILE 'HOME' ENTERED AT 11:59:19 ON 12 SEP 2001) FILE 'REGISTRY' ENTERED AT 11:59:24 ON 12 SEP 2001 L1STRUCTURE UPLOADED L2OUE L1 L3 20 S L2 FILE 'STNGUIDE' ENTERED AT 12:00:33 ON 12 SEP 2001 FILE 'REGISTRY' ENTERED AT 12:08:23 ON 12 SEP 2001 399 S L2 SSS FUL L4FILE 'CAPLUS' ENTERED AT 12:08:34 ON 12 SEP 2001 L5 102 S L4 FILE 'REGISTRY' ENTERED AT 12:09:30 ON 12 SEP 2001 10 S BISPIDINE L6 L7 505 S C7H14N2/MF Г8 1 S L7 AND L6 L9 2255 S 354.23?/RID FILE 'CAPLUS' ENTERED AT 12:15:24 ON 12 SEP 2001 76 S L5 AND JOURNAL/DT L10 L114 S L10 AND 2000/SO L12 5 S L10 AND 2001/SO

=> d bib abs hitstr 113 1-97

97 S L5 NOT L12

3 ANSWER 1 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 2001:537517 CAPLUS

DN 135:123343

TI Preparation of thiolamide curing agents

IN Krebaum, Paul

PA Molex Incorporated, USA

SO U.S., 6 pp. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

PΙ

PATENT NO. KIND DATE APPLICATION NO. DATE
US 6265519 B1 20010724 US 1998-206821 19981208

OS MARPAT 135:123343

AB Present invention relates to thiolamide curing agents and methods for their prepn. and use. The thiolamide curing agents are the reaction product of a thiol contg. compd. and an amine contg. compd. Thus, 800 g Jeffamine T 3000 and 80 g 3-mercaptopropionic acid were reacted in the presence of Tyzor TBT and anhyd. methanesulfonic acid in toluene to give a thiolamide curing agent. Bisphenol F epoxy resin (3.5 g) was set to a gel within 10 min in the presence of 25 g thiolamide curing agent and 0.5 g diazabicycloundecene.

IT 280-74-0, 3,7-Diazabicyclo[3.3.1]nonane RL: CAT (Catalyst use); USES (Uses)

(catalyst; prepn. of thiolamide curing agents)

RN 280-74-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)

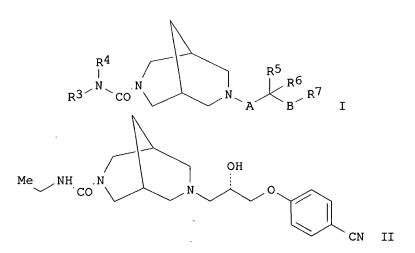


RE.CNT 11

RE

- (2) Armbruster; US 4894431 1990 CAPLUS
- (3) Cantor; US 5703138 1997 CAPLUS
- (4) Cantor; US 5712321 1998 CAPLUS
- (5) Giovando; US 5310826 1994 CAPLUS
- (6) Goel; US 4696992 1987 CAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 2 OF 97 CAPLUS COPYRIGHT 2001 ACS
      2000:900637 CAPLUS
AN
DN
      134:56700
      Preparation of new bispidines useful in the treatment of cardiac
ΤI
      arrhythmias
      Alstermark, Christer; Andersson, Kjell; Bjore, Annika; Bjorsne, Magnus;
IN
      Lindstedt, Alstermark Eva-Lotte; Nilsson, Goran; Polla, Magnus;
      Strandlund, Gert; Ortengren, Ylva
      Astrazeneca AB, Swed.
SO
      PCT Int. Appl., 130 pp.
      CODEN: PIXXD2 .
DT
      Patent
      English
LΑ
FAN.CNT 1
      PATENT NO.
                          KIND
                                  DATE
                                                    APPLICATION NO.
·PΙ
      WO 2000077000
                                  20001221
                                                    WO 2000-SE1254
                                                                         20000615
                           Α1
               AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
                CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
               ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
           RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
                DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
                CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI SE 1999-2268
                                 19990616
                           Α
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MARPAT 134:56700

OS GI

AB Bispidines, such as I [R3 = H, alkyl; R4 = H, alkyl, alkoxy; NR3R4 = heterocyclyl; R5 = H, halogen, alkyl, alkoxy, acyloxy, alkylsulfonyloxy, carbamoyl, etc.; R6 = H, alkyl; R5R6 = O; R7 = alkyl, aryl, heterocyclyl; A, B = bond, linking group, such as alkylene, etc.], were prepd. for pharmaceutical use in the treatment of cardiac arrhythmias, in particular atrial and ventricular arrhythmias. Thus, bispidine II was prepd. with

51% yield by amidation of (S)-4-[3-(3,7-diazabicyclo[3.3.1]non-3-y1)-2-hydroxypropoxy]benzonitrile with Et isocyanate. The prepd. bispidines were tested for primary electrophysiol. effects in anesthetized guinea pigs.

IT 313475-71-7P 313475-73-9P 313475-75-1P 313475-77-3P 313475-79-5P 313475-82-0P 313475-84-2P 313475-86-4P 313475-88-6P 313475-90-0P 313475-92-2P 313475-95-5P 313475-97-7P 313476-02-7P 313476-05-0P 313476-07-2P 313476-09-4P 313476-11-8P 313476-13-0P 313476-15-2P 313476-18-5P 313476-20-9P 313476-23-2P 313476-31-2P 313476-31-2P 313476-34-5P 313476-37-8P 313476-39-0P 313476-41-4P 313476-43-6P 313476-44-7P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of new bispidines useful in the treatment of cardiac arrhythmias)

RN 313475-71-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313475-73-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-(cyclopropylmethyl)- (9CI) (CA INDEX NAME)

RN 313475-75-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-ethanol, .alpha.-[(4-cyanophenoxy)methyl]-7-(4-morpholinylcarbonyl)-, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313475-77-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-[(methylsulfonyl)amino]propyl]-N-ethyl- (9CI) (CA INDEX NAME)

RN 313475-79-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313475-82-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[(2R)-3-[4-cyano-2-[[(2-cyanoethyl)amino]carbonyl]phenoxy]-2-hydroxypropyl]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313475-84-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[(2S)-3-[4-cyano-2-[(cyclopropylamino)carbonyl]phenoxy]-2-hydroxypropyl]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313475-86-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-ethyl-7-[2-(4-nitrophenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \\ \parallel & \\ \text{EtNH-C} & \\ & N \\ \hline & N \\ \hline & \text{CH}_2 \\ \hline & \text{CH}_2 \\ \hline \end{array}$$

RN 313475-88-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(cyanomethyl)-7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313475-90-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-ethyl-7-[2-[4-[(methylsulfonyl)amino]phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 313475-92-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-fluoropropyl]-N-ethyl- (9CI) (CA INDEX NAME)

EtNH-C
$$N$$
 N $CH_2-CH-CH_2-O$ CN

RN 313475-95-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-[2-oxo-2-(propylamino)ethyl]- (9CI) (CA INDEX NAME)

RN 313475-97-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-[(4-morpholinylcarbonyl)amino]propyl]-N-ethyl- (9CI) (CA INDEX NAME)

RN 313475-99-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-[2-(4-cyanophenyl)ethyl]-7-(4-oxoheptyl)- (9CI) (CA INDEX NAME)

RN 313476-02-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(4-oxoheptyl)-, 2-(4-cyanobenzoyl)hydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ N-Pr-C-(CH_2) & 3 \\ \hline & N-C-NH-NH-C \end{array}$$

RN 313476-05-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-ethanamine, .alpha.-[(4-cyanophenoxy)methyl]-7-(1-piperidinylcarbonyl)- (9CI) (CA INDEX NAME)

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09/623,726

RN 313476-07-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-ethyl-7-[2-hydroxy-3-[4-(1H-imidazol-1-yl)phenoxy]propyl]- (9CI) (CA INDEX NAME)

EtNH-C OH OH N N
$$\sim$$
 CH₂-CH-CH₂-O

RN 313476-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-[3-(4-cyanophenoxy)propyl]-7-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

$$N - CH_2 - CH_2$$
 $N - C - NH - (CH_2)_3 - O$
 CN

RN 313476-11-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 313476-13-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-2-propenyl- (9CI) (CA INDEX NAME)

$$H_2C = CH - CH_2 - NH - C$$
 N
 $N - CH_2 - CH - CH_2 - O$
 $N - CH_2 - CH - CH_2 - O$

RN 313476-15-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-[2-(2-thienyl)ethyl]- (9CI) (CA INDEX NAME)

RN 313476-18-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-[3-(ethylamino)-3-oxopropyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ \parallel & \parallel & \\ E + NH - C - CH_2 - CH_2 - NH - C \\ \hline & N & OH \\ N - CH_2 - CH - CH_2 - O \\ \end{array}$$

RN 313476-20-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(1-cyanoethyl)-7-[3-(4-cyanophenoxy)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

RN 313476-23-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

$$F_3C-CH_2-NH-C$$

$$N$$

$$OH$$

$$CH_2-CH-CH_2-O$$

$$CN$$

RN 313476-26-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-[2-oxo-2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 313476-28-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-1,3-benzodioxol-5-yl-7-[3-(4-cyanophenoxy)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

RN 313476-29-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-[(4-cyanophenyl)amino]propyl]-N-[2-oxo-2-(propylamino)ethyl]- (9CI) (CA INDEX NAME)

RN 313476-31-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[4-(4-cyanophenyl)-4-(3,4-dimethoxyphenoxy)butyl]-N-ethyl- (9CI) (CA INDEX NAME)

RN 313476-34-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-[4-cyano-2-

[(cyclopropylamino)carbonyl]phenoxy]-2-hydroxypropyl]-N-phenyl- (9CI) (CA INDEX NAME)

RN 313476-37-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(4-cyanophenyl)-7-[3-(ethylsulfonyl)propyl]- (9CI) (CA INDEX NAME)

RN 313476-39-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-[(2-cyano-1H-indol-4-yl)oxy]-2-hydroxypropyl]-N-phenyl- (9CI) (CA INDEX NAME)

RN 313476-41-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[(7-cyano-2,3-dihydro-1,4-benzodioxin-2-yl)methyl]-N-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 313476-43-6 CAPLUS

Page 12



CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[[(2S)-6-cyano-3,4-dihydro-4-(methylsulfonyl)-2H-1,4-benzoxazin-2-yl]methyl]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313476-44-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[2-[[[4,5-bis(4-cyanophenyl)-1H-pyrazol-1-yl]acetyl]amino]ethyl]-N-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C & O & O & O \\ \hline & N & O & O \\ N & N & CH_2-CH_2-NH-C-CH_2-N \\ \hline & & CN & CN \\ \end{array}$$

IT 227939-99-3 313477-26-8 313477-39-3

RL: RCT (Reactant)

(prepn. of new bispidines useful in the treatment of cardiac arrhythmias)

RN 227939-99-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313477-26-8 CAPLUS

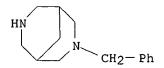
CN Benzonitrile, 4-[(2S)-3-(3,7-diazabicyclo[3.3.1]non-3-yl)-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313477-39-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)-7-(1-piperidinylcarbonyl)-(9CI) (CA INDEX NAME)

IT 69407-32-5P 122455-64-5P 122455-81-6P 227940-70-7P 227940-71-8P 227940-72-9P 227940-73-0P 312955-28-5P 313476-52-7P 313476-53-8P 313476-54-9P 313476-55-0P 313476-56-1P 313476-63-0P 313476-65-2P 313476-70-9P 313476-71-0P 313476-74-3P 313476-76-5P 313476-77-6P 313476-86-7P, 3,7-Diazabicyclo[3.3.1] nonane-3-ethanol 313476-88-9P 313476-91-4P 313476-93-6P 313476-94-7P 313477-00-8P 313477-03-1P 313477-05-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of new bispidines useful in the treatment of cardiac arrhythmias) RN69407-32-5 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 122455-64-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-phenyl-7-(phenylmethyl)-(9CI) (CA INDEX NAME)

RN 122455-81-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-phenyl- (9CI) (CA INDEX NAME)

RN 227940-70-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-oxo-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-71-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-72-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

09/623,726

RN 227940-73-0 CAPLUS

CN Benzonitrile, 4-[3-(3,7-diazabicyclo[3.3.1]non-3-yl)-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

RN 312955-28-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-(3,4-dimethoxyphenoxy)butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313476-52-7 CAPLUS

CN Methanesulfonamide, N-[2-(4-cyanophenoxy)-1-(3,7-diazabicyclo[3.3.1]non-3-ylmethyl)=(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \parallel \\ NH-S-Me \\ \parallel \\ O \\ N-CH_2-CH-CH_2-O \end{array}$$

RN 313476-53-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(1-methylethyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

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COLOR THE PROPERTY OF

RN 313476-54-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 313476-55-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-ethyl-7-(phenylmethyl)-(9CI) (CA INDEX NAME)

RN 313476-56-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & & \\ & \text{C-NHEt} \\ & \text{O} \end{array}$$

RN 313476-63-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-N-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & OH & OH \\ \hline N & OH & CH_2-CH-CH_2-O \end{array}$$

RN 313476-65-2 CAPLUS

CN Glycine, N-[[7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-3,7-diazabicyclo[3.3.1]non-3-yl]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 313476-70-9 CAPLUS

CN Carbamic acid, [2-(4-cyanophenoxy)-1-[[7-[(ethylamino)carbonyl]-3,7-diazabicyclo[3.3.1]non-3-yl]methyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313476-71-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[2-amino-3-(4-cyanophenoxy)propyl]-N-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C} & \text{C} & \text{C} \\ & \text{C} & \text{NH}_2 \\ & \text{N} & \text{CH}_2 - \text{CH} - \text{CH}_2 - \text{O} \end{array}$$

RN 313476-74-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-[3-(2-propyl-1,3-dioxolan-2-yl)propyl]-(9CI) (CA INDEX NAME)

09/623,726

RN 313476-76-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-piperidinylcarbonyl)- (9CI) (CA INDEX NAME)

RN 313476-77-6 CAPLUS

CN Carbamic acid, [1-[(4-cyanophenoxy)methyl]-2-[7-(1-piperidinylcarbonyl)-3,7-diazabicyclo[3.3.1]non-3-yl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313476-86-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-ethanol (9CI) (CA INDEX NAME)

$$^{\rm HN}$$
 $^{\rm N}$ $^{\rm CH_2-CH_2-OH}$

RN 313476-88-9 CAPLUS

CN :beta.-Alanine, N-[[7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-3,7-diazabicyclo[3.3.1]non-3-yl]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ \parallel & \parallel & O \\ C-CH_2-CH_2-NH-C & OH & OH \\ N-CH_2-CH-CH_2-O & OH \\ N-CH_2-CH-CH_2-O & OH \\ \end{array}$$

RN 313476-91-4 CAPLUS

Page 19

CN Glycine, N-[[7-(phenylmethyl)-3,7-diazabicyclo[3.3.1]non-3-yl]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 313476-93-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-[2-oxo-2-(propylamino)ethyl]-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 313476-94-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-[2-oxo-2-(propylamino)ethyl]- (9CI) (CA INDEX NAME)

RN 313477-00-8 CAPLUS

CN Benzonitrile, 4-[4-(3,7-diazabicyclo[3.3.1]non-3-yl)-1-(3,4-dimethoxyphenoxy)butyl]- (9CI) (CA INDEX NAME)

RN 313477-03-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[[(4-cyanophenyl)amino]carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313477-05-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(4-cyanophenyl)- (9CI) (CA INDEX NAME)

RE.CNT 5

RE

- (1) Astra Aktiebolag; WO 9931100 A1 1999 CAPLUS
- (2) Basf Aktiengesellschaft; EP 0308843 A2 1989 CAPLUS
- (3) Kali-Chemie Pharma Gmbh; EP 0306871 A2 1989 CAPLUS
- (4) Kenneth, D; US 5786481 A 1998 CAPLUS
- (5) The Board Of Regents Of Oklahoma State University; WO 9107405 A1 1991 CAPLUS

```
ANSWER 3 OF 97 CAPLUS COPYRIGHT 2001 ACS
     2000:900636 CAPLUS
DN
     134:42151
ΤI
     Preparation of new bispidines useful in the treatment of cardiac
IN
     Bjore, Annika; Bjorsne, Magnus; Halvarsson, Torbjorn; Hoffmann,
     Kurt-jurgen; Samuelsson, Bertil; Strandlund, Gert
PA
     Astrazeneca Ab, Swed.
SO
     PCT Int. Appl., 87 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                        KIND
                               DATE
                                               APPLICATION NO.
PI
     WO 2000076999
                         Α1
                               20001221
                                             . WO 2000-SE1253
                                                                 20000615
              AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
              CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
              LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
              SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
              ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
              DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
              CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI SE 1999-2270
                              19990616
                         Α
OS
     MARPAT 134:42151
GΙ
```

$$R^2$$
 R^3
 R^5 ?
 R^6
 R^6

AB Bispidines, such as I [R1 = alkyl, arylalkyl, etc.; R2, R3 = H, OH, alkyl, etc.; R2R3 = O; R4, R5a, R5b = H, alkyl; R6 = OH, CN, NO2, NH2, halogen, etc.; X = O, S; A, B = bond, linking group, such as alkylene, etc.; D = H, OH, alkyl, aminoalkyl, etc.], were prepd. for pharmaceutical use in the treatment of cardiac arrhythmias, in particular atrial and ventricular

arrhythmias. Thus, bispidine II was prepd. in multistep synthetic sequence starting from Et 4-oxo-1-piperidinecarboxylate, epichlorohydrin, and 4-cyanophenol. The prepd. bispidines were tested for primary electrophysiol. effects in anesthetized guinea pigs.

IT 313238-19-6P

RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of new bispidines useful in the treatment of cardiac arrhythmias)

RN 313238-19-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-amino-2-(4-cyanophenyl)ethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

IT 313238-07-2P 313238-09-4P 313238-13-0P

313238-15-2P 313238-17-4P 313238-21-0P

313238-23-2P 313238-25-4P 313238-26-5P

313238-28-7P 313238-30-1P 313269-42-0P

313269-43-1P 313269-44-2P 313269-45-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of new bispidines useful in the treatment of cardiac arrhythmias)

RN 313238-07-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-9-hydroxy-, ethyl ester, (9-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 313238-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-9-hydroxy-, 1,1-dimethylethyl ester, (9-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 313238-13-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-(benzoyloxy)-7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester, (9-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 313238-15-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-9-(1-oxopropoxy)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-17-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[(4-cyanophenyl)amino]propyl]-9-hydroxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C N (CH₂)
$$_3$$
-NH CN

Page 24

RN 313238-21-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2[(aminocarbonyl)amino]-2-(4-cyanophenyl)ethyl]-, 1-methylethyl ester (9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} O & O & O \\ I-PrO-C & N & NH-C-NH_2 \\ N & CH_2-CH & CN \end{array}$$

RN 313238-23-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-[(aminooxoacetyl)amino]-2-(4-cyanophenyl)ethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \parallel & \parallel \\ \text{i-PrO-C} \\ N & \text{NH-C-C-NH}_2 \\ \text{CN} \\ \end{array}$$

RN 313238-25-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-(4-cyanophenyl)-2-(formylamino)ethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 313238-26-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-amino-3-(4-cyanophenoxy)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C
$$NH_2$$
 NH_2 NH_2

RN 313238-28-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-amino-3-(4-cyanophenoxy)propyl]-9-hydroxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-30-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[(4-cyanophenyl)amino]propyl]-9-hydroxy-1,5-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313269-42-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-9-hydroxy-, ethyl ester, (9-anti)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 313269-43-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-9-hydroxy-, 1,1-dimethylethyl ester, (9-anti)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 313269-44-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-9-hydroxy-9-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 313269-45-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-(benzoyloxy)-7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester, (9-anti)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 69407-32-5P 227940-23-0P 227940-70-7P 227940-71-8P 227940-72-9P 227940-74-1P 227940-75-2P 227940-78-5P 313238-37-8P 313238-39-0P 313238-42-5P 313238-44-7P 313238-46-9P 313238-48-1P 313238-51-6P 313238-53-8P 313238-63-0P 313238-65-2P

313238-75-4P 313238-77-6P 313238-79-8P 313238-81-2P 313238-83-4P 313269-46-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of new bispidines useful in the treatment of cardiac arrhythmias)

RN 69407-32-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{HN} \\ \text{N} \\ \text{CH}_2\text{--Ph} \end{array}$$

RN 227940-23-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-(4-cyanophenyl)-2-hydroxyethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

$$i-Pro-C$$
 N
 N
 CH_2
 CH

RN 227940-70-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-oxo-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-71-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-72-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 1,1-dimethylethyl ester

09/623,726

(9CI) (CA INDEX NAME)

RN 227940-74-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 227940-75-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 227940-78-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-9-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 313238-37-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-hydroxy-9-methyl-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-39-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-hydroxy-9-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Me
$$C-OBu-t$$

RN 313238-42-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]-9-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-44-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]-9-hydroxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-46-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-(benzoyloxy)-7-[3-(4-cyanophenoxy)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]-, 1,1-dimethylethyl ester, (9-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 313238-48-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]-9-(1-oxopropoxy)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-51-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-hydroxy-7- (phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-53-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-hydroxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-63-0 CAPLUS

09/623,726

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-chloro-2-(4-cyanophenyl)ethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 313238-65-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-azido-2-(4-cyanophenyl)ethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

$$i\text{-PrO-C} \\ N \\ N \\ CH_2 \\ CH$$

RN 313238-75-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-[[(phenylmethoxy)carbonyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-77-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-[[(phenylmethoxy)carbonyl]amino]propyl]-9-hydroxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-79-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 1,5-dimethyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

09/623,726

RN 313238-81-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-hydroxy-1,5-dimethyl-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313238-83-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-hydroxy-1,5-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313269-46-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-(benzoyloxy)-7-[3-(4-cyanophenoxy)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]-, 1,1-dimethylethyl ester, (9-anti)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 5

RE

- (1) Astra Aktiebolag; WO 9931100 A1 1999 CAPLUS(2) Basf Aktiengesellschaft; EP 0308843 A2 1989 CAPLUS
- (3) Kali-Chemie Pharma Gmbh; EP 0306871 A2 1989 CAPLUS
- (4) Kenneth, D; US 5786481 A 1998 CAPLUS
- (5) The Board Of Regents Of Oklahoma State University; WO 9107405 A1 1991 CAPLUS

```
ANSWER 4 OF 97 CAPLUS COPYRIGHT 2001 ACS
     2000:900635 CAPLUS
     134:42150
ΤI
     Preparation of new bispidines useful in the treatment of cardiac
     arrhythmias
IN
     Bjorsne, Magnus; Frantsi, Marianne; Hoffmann, Kurt-Jurgen; Ohlsson, Bengt
     Astrazeneca AB, Swed.
PA
     PCT Int. Appl., 76 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                            APPLICATION NO.
                                                             DATE
     WO 2000076998
                            20001221
                                           WO 2000-SE1252
ΡI
                       Α1
                                                             20000615
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
             SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
             ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI SE 1999-2269
                       Α
                            19990616
OS
    MARPAT 134:42150
GΙ
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$$R^{2}$$
 R^{3}
 R^{5}
 R^{5}

AB Bispidines, such as I [R1 = alkyl, arylalkyl, etc.; R2, R3, R5a, R5b, R5c, R5d, R5e, R5f = H, alkyl; R6 = OH, CN, NO2, NH2, halogen, etc.; R9 = alkyl, aryl, acyl, etc.; X = O, S; A, B = bond, linking group, such as alkylene, etc.; D = OH, alkyl, etc.], were prepd. for pharmaceutical use in the treatment of cardiac arrhythmias, in particular atrial and

ventricular arrhythmias. Thus, bispidine II was prepd. in multistep synthetic sequence starting from N,N'-dibenzylbispidine, 4-cyanophenol, and epichlorohydrin. The prepd. bispidines were tested for primary electrophysiol. effects in anesthetized guinea pigs.

IT 312961-89-0P 312961-90-3P 312961-91-4P 313056-94-9P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of new bispidines useful in the treatment of cardiac arrhythmias)

RN 312961-89-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-2,4-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 312961-90-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-6,8-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C
$$N$$
 N N $CH_2-CH-CH_2-O$ N Me N

RN 312961-91-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-6-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 313056-94-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-6,8-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 69407-32-5P 227940-71-8P 312961-92-5P 312961-93-6P 312961-95-8P 312961-96-9P 312961-98-1P 312961-99-2P 313056-95-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of new bispidines useful in the treatment of cardiac arrhythmias)

RN 69407-32-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 227940-71-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 312961-92-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 2-methyl-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Ph-CH_2 \\ \hline \\ N \\ \hline \\ N \\ C-OBu-t \\ \\ Me \\ O \end{array}$$

Page 37

RN 312961-93-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 2,4-dimethyl-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 312961-95-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 2,4-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 312961-96-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4-dimethyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 312961-98-1 CAPLUS

CN Benzonitrile, 4-[3-(2,4-dimethyl-3,7-diazabicyclo[3.3.1]non-3-yl)-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

RN 312961-99-2 CAPLUS

CN Benzonitrile, 4-[2-hydroxy-3-(2-methyl-3,7-diazabicyclo[3.3.1]non-3-yl)propoxy]- (9CI) (CA INDEX NAME)

RN 313056-95-0 CAPLUS

CN Benzonitrile, 4-[(2S)-3-(2,4-dimethyl-3,7-diazabicyclo[3.3.1]non-3-yl)-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 5

RE

- (1) Astra Aktiebolag; WO 9931100 A1 1999 CAPLUS
- (2) Basf Akatiengesellschaft; EP 0308843 A2 1989 CAPLUS
- (3) Kali-Chemie Pharma Gmbh; EP 0306871 A2 1989 CAPLUS
- (4) Kenneth, D; US 5786481 A 1998 CAPLUS
- (5) The Board Of Regents Of Oklahoma State University; WO 9107405 A1 1991 CAPLUS

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09/623,726
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ANSWER 5 OF 97 CAPLUS COPYRIGHT 2001 ACS
AN
     2000:900634 CAPLUS
DN
     134:42149
ΤI
     Preparation of new bispidines useful in the treatment of cardiac
     arrhythmias
IN
     Frantsi, Marianne; Hoffmann, Kurt-Jurgen; Strandlund, Gert
PA
     Astrazeneca AB, Swed.
SO
     PCT Int. Appl., 60 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                            APPLICATION NO.
     WO 2000076997
                            20001221
                                           WO 2000-SE1251
                                                             20000615
PΙ
                       A1
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
             SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
             ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI SE 1999-2271
                       Α
                            19990616
     CASREACT 134:42149; MARPAT 134:42149
OS
GI
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$$R^2$$
 R^3
 R^5 ?
 R^6
 R^4
 R^6
 R^6

AB Bispidines, such as I [R1 = alkyl, arylalkyl, etc.; R2, R3, R4, R5a, R5b = H, alkyl; R6 = OH, CN, NO2, NH2, halogen, etc.; R9 = alkyl, aryl, acyl, etc.; X = O, S; A, B = bond, linking group, such as alkylene, etc.], were prepd. for pharmaceutical use in the treatment of cardiac arrhythmias, in particular atrial and ventricular arrhythmias. Thus, bispidine II was prepd. in multistep synthetic sequence starting from N,N'-

Page 40

1 6 4 May 2 3 1 3 1 1 5

dibenzylbispidine, 4-(1-hydroxy-3-butenyl)benzonitrile, and 3,4-dimethoxyphenol. The prepd. bispidines were tested for primary electrophysiol. effects in anesthetized guinea pigs.

IT 312955-28-5P 312955-29-6P 312955-30-9P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of bispidines useful in the treatment of cardiac arrhythmias)

RN 312955-28-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-(3,4-dimethoxyphenoxy)butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 312955-29-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-(4-hydroxyphenoxy)butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 312955-30-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-(4-pyridinylmethoxy)butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C N N (CH₂) 3-CH CN
$$CH_2$$

IT 69407-32-5P 227940-28-5P 227940-71-8P 227940-72-9P 227940-94-5P 312955-35-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of bispidines useful in the treatment of cardiac arrhythmias)

RN 69407-32-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \\ & &$$

RN 227940-28-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-hydroxybutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-71-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-72-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-94-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 312955-35-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenoxy]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RE.CNT 5

RE

- (1) Astra Aktiebolag; WO 9931100 A1 1999 CAPLUS
- (2) Basf Aktiengesellschaft; EP 0308843 A2 1989 CAPLUS
- (3) Kali-Chemie Pharma Gmbh; EP 0306871 A2 1989 CAPLUS
- (4) Kenneth, D; US 5786481 A 1998 CAPLUS

(5) The Board Of Regents Of Oklahoma State University; WO 9107405 A1 1991 CAPLUS

LX

ANSWER 6 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN \2000:780169 CAPLUS

DN 134:85911

TI 1H NMR spectral study of some 4-hydroxy-2,6-diphenylpiperidines and a systematic analysis of 1H chemical shifts in some piperidines and 3,7-diazabicyclo[3.3.1]nonane derivatives

AU Pandiarajan, K.; Manimekalai, A.; Rajarajan, G.

CS Department of Chemistry, Annamalai University, Annamalai Nagar, 608 002, India

SO Indian J. Chem., Sect. B: Org. Chem. Incl. Med. Chem. (2000), 39B(7), 517-524

CODEN: IJSBDB; ISSN: 0376-4699

PB National Institute of Science Communication, CSIR

DT Journal

LA English

AB 1H NMR spectra have been recorded for some 3,5-dimethyl-2,6-diphenyl-4-piperidinol derivs. and their corresponding axial 4-hydroxy epimers. The proton chem. shifts and coupling consts. have been detd. by anal. of the spectra. The vicinal coupling consts. suggest that a boat form may make a slight contribution to the equatorial alcs. The .DELTA..delta.ea value for the protons in 5-position is less in the axial alc. than in the corresponding equatorial alc. and becomes neg. in one case. The effects of Me, Et, iso-Pr and hydroxyl groups on the chem. shifts of the ring protons are discussed. Anal. of the chem. shifts of some 9-hydroxy-3,7-diazabicyclo[3.3.1]nonanes suggests that the 3,7-di-Ph substituted compds. exist in a boat-chair conformation.

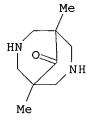
IT 80808-96-4

RL: PRP (Properties)

(proton NMR study of some piperidinols and diazabicyclononane derivs.)

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)



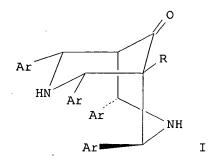
RE.CNT 34

RE

- (1) Arumugam, N; Magn Reson Chem 1987, V25, P869 CAPLUS
- (2) Balasubramanian, M; Tetrahedron 1963, V19, P2135 CAPLUS
- (3) Balasubramanian, M; Tetrahedron Lett 1960, P23 CAPLUS
- (4) Baliah, V; Chem Rev 1983, V83, P379 CAPLUS
- (7) Bhavani, N; Magn Reson Chem 1996, V34, P582 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 7 OF 97 CAPLUS COPYRIGHT 2001 ACS
     2000:757308 CAPLUS
     134:42298
     NMR study of the stereochemistry of 2,4,6,8-tetraaryl-3,7-
     diazabicyclo[3.3.1]nonan-9-ones
     Vijayakumar, V.; Sundaravadivelu, M.; Perumal, S.; Hewlins, M. J. E.
ΑU
     Department of Chemistry, Gandhigram Rural Institute (Deemed University),
CS
     Gandhigram, 624 302, India
    Magn. Reson. Chem. (2000), 38(10), 883-885
SO
     CODEN: MRCHEG; ISSN: 0749-1581
PB
     John Wiley & Sons Ltd.
DT
     Journal
LΑ
     English
GΙ
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The 1H and 13C NMR spectra of 2,4,6,8-tetraaryl-3,7-diazabicyclo[3.3:1]nonan-9-ones [I; Ar = Ph, R = H (II); Ar = p-CH3C6H4, R = H (III); Ar = p-CH3OC6H4, R = H (IV); Ar = Ph, R = CH3 (V)] were measured at 360 and 90 MHz, resp. The chem. shifts for II-V were assigned unambiguously using one- and two-dimensional NMR spectroscopic data and nuclear Overhauser enhancement studies. These results clearly indicate a chair-boat conformation for these compds. with (i) all aryl groups orientated equatorially and (ii) the aryl groups of the boat lying in the shielding zone of the aryl groups of the chair. Literature assignments of carbon chem. shifts were also revised.

Relative stereochemistry.

RN 75549-52-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methylphenyl)-, (2R,4S,6S,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 142698-37-1 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl-, (2R,4R,6R,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Page 47

RN 312583-40-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methoxyphenyl)-, (2R,4S,6S,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 12

RE

(1) Azerbaev, I; Vestn Akad Kaz SSR 1975, V47 CAPLUS

(2) Baliah, V; Indian J Chem, Sect B 1977, V15, P684 CAPLUS

(3) Binning, F; DE 2726571 1978 CAPLUS

(4) Chiavarelli, S; Ann 1st Supersanita 1972, V8, P156 CAPLUS

(5) Hart, N; Aust J Chem 1967, V20, P561 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 8 OF 97 CAPLUS COPYRIGHT 2001 ACS
       2000:742083 CAPLUS
       133:309908
DN
       Preparation of piperazinyladamantylmethylbenzamides and related compounds
ΤI
       as P2X7 receptor antagonists.
       Alcaraz, Lilian; Furber, Mark; Mortimore, Michael
IN
       AstraZeneca AB, Swed.
PA
       PCT Int. Appl., 166 pp.
SO
       CODEN: PIXXD2
DT
       Patent
       English
LΑ
FAN.CNT 1
                                                               APPLICATION NO.
       PATENT NO.
                                KIND
                                         DATE
                                         20001019
                                                               WO 2000-SE663
PΙ
       WO 2000061569
                                A1
                                                                                         20000406
                   AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
                   CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
                   ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LD, LD, LN, LS, GF, KE, KG, KF, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI SE 1999-1270
                                 Α
                                         19990409
                                         20000201
       GB 2000-2330
                                  Α
       MARPAT 133:309908
OS
GΙ
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$$(CH_2)_{m}AAr$$

$$R^{1}$$

$$R^{1}$$

$$R^{1}$$

$$R^{2}$$

$$Q^{2} = R^{2}$$

$$R^{2}$$

$$R^{2}$$

$$R^{2}$$

$$R^{3}$$

$$R^{4}$$

$$R^{3}$$

$$R^{4}$$

$$R^{2}$$

$$R^{2}$$

$$R^{2}$$

AB Title compds. I [m = 1-3; R1 = H, halo; A = CONH; Ar = Q1, Q2; X = O, CO, (CH2)1-6, S, SO, SO2, etc.; 1 of R2, R3 = halo, cyano, NO2, amino, OH, (substituted) alkyl, cycloalkyl, alkoxy, etc., the other = H, halo; R4 = 3-9 membered (unsatd.) (substituted) heterocyclyl contg. 1-2 N atoms, substituted 3-8 membered carbocyclyl], were prepd. Thus, 3-chloro-2-nitro-N-[tricyclo[3.3.1.13,7]dec-1-ylmethyl]benzamide (prepn. given) and tert-Bu piperazine-1-carboxylate were heated at 120.degree. in Me2SO for 24 h to give the coupling product, which was stirred with HCl in THF/dioxane to give 2-nitro-3-piperazin-1-yl-N-[tricyclo[3.3.1.13,7]dec-1-ylmethyl]benzamide. I antagonized P2X7 receptors with pIC50 >4.50.

IT 301672-21-9P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of piperazinyladamantylmethylbenzamides and related compds. as P2X7 receptor antagonists)

RN 301672-21-9 CAPLUS

CN Benzamide, 2-chloro-5-(3,7-diazabicyclo[3.3.1]non-3-ylmethyl)-N(tricyclo[3.3.1.13,7]dec-1-ylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

NAME)

O

C-NH-CH2

C1

HCl

RE.CNT 4

RE

- (1) Astra Pharmaceuticals Ltd; WO 9929660 A1 1999 CAPLUS
- (2) Astra Pharmaceuticals Ltd; WO 9929661 A1 1999 CAPLUS
- (3) Bernstein; US 3789072 A 1974 CAPLUS
- (4) Kyowa Hakko Kogyo Co Ltd; EP 0395093 A1 1990 CAPLUS

09/623,726 ANSWER 9 OF 97 CAPLUS COPYRIGHT 2001 ACS 2000:535147 CAPLUS 133:135332 ΤI Preparation of diazabicyclic derivatives as nicotinic acetylcholine receptor ligands Bunnelle, William H.; Cristina, Daniela Barlocco; Daanen, Jerome F.; Dart, IN Michael J.; Meyer, Michael D.; Ryther, Keith B.; Schrimpf, Michael R.; Sippy, Kevin B.; Toupence, Richard B. PA Abbott Laboratories, USA SO PCT Int. Appl., 123 pp. CODEN: PIXXD2 DTPatent LΑ English FAN.CNT 1

Patent
English
NT 1
PATENT NO. KIND DATE APPLICATION NO.

______ WO 2000044755 20000803 PΙ **A**1 WO 2000-US1620 20000125 W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

DATE

PRAI US 1999-239838 A 19990129

OS MARPAT 133:135332

GI

The title compds. (I) [wherein V and X = independently a bond or CH2; W AΒ and Y = independently a bond, CH2, or CH2CH2; Z = CH2, CH2CH2, or CH2CH2CH2; L1 = a bond or (CH2)n; n = 1-5; R1 = certain heteroarom. rings, such as pyridinyl, pyrimidinyl, pyrazinyl, quinolinyl, etc.; R2 = H, alkoxycarbonyl, (amino)alkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy(alkyl), phenoxycarbonyl, or NH2] and their pharmaceutically acceptable salts were prepd. as cholinergic modulators for the treatment of pain and other conditions. For example, (-)-II.bul.Ts-OH was prepd. in a multi-step sequence involving N-protection of (1R,4R)-2-benzyl-2,5diazabicyclo[2.2.1]heptane.bul.2HBr with CO(OBu-t)2 (94%), debenzylation (93%), addn. of 2-chloro-5-iodopyridine (67%), and deprotection followed by salt formation (71%). (-)-II.bul.Ts-OH exhibited high affinity for the nicotinic acetylcholine receptor with Ki of 0.01 nM and showed a significant antinociceptive effect at the minimally ED of 0.62 .mu.mol/kg in the mouse hot plate paradigm.

IT 280-74-0, 3,7-Diazabicyclo[3.3.1] nonane

RL: RCT (Reactant)

(prepn. of N-substituted diazabicycloalkanes as nicotinic acetylcholine receptor ligands by addn. of haloheterocycles to protected

diazabicyloalkanes followed by deprotection and optional substitution) 280-74-0 CAPLUS RN

3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME) CN



RE.CNT

RE

- (1) Daniela, B; JOURNAL OF MEDICINAL CHEMISTRY 1998, V41(5), P674
- (2) Eugene, T; US 5478939 A 1995 CAPLUS
- (3) Neurosearch AS; WO 9854181 A 1998 CAPLUS
- (4) Neurosearch AS; WO 9854182 A 1998 CAPLUS

ANSWER 10 OF 97 CAPLUS COPYRIGHT 2001 ACS

An 2000:528840 CAPLUS

DN 133:281938

TI Bispidine-derived N-acyliminium ions in synthesis: stereocontrolled construction of the BCD rings of sparteine

AU Harrison, J. R.; O'Brien, P.

CS Department of Chemistry, University of York, Heslington, York, YO10 5DD,

UK

Tetrahedron Lett. (2000), 41(32), 6167-6170

CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 133:281938

GΙ

AB Reaction of Grignard reagents with bispidine-derived N-acyliminium ions I (generated in situ from an .alpha.-methoxy bispidine amide II) has been studied as a new route to sparteine analogs. The addn. reactions proceed with complete diastereoselectivity to generate products with the same relative stereochem. as in the BCD rings of sparteine. Stereocontrolled synthesis of a tricyclic diamine structurally equiv. to the BCD rings of sparteine, is described.

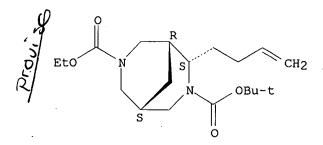
IT 300543-06-0P 300543-07-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (bispidine-derived N-acyliminium ions in stereocontrolled construction of the BCD rings of sparteine synthesis)

RN 300543-06-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 2-(3-butenyl)-, 3-(1,1-dimethylethyl) 7-ethyl ester, (1R,2S,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 300543-07-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 2-(4-hydroxybutyl)-,

Page 53

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3-(1,1-dimethylethyl) 7-ethyl ester, (1R,2S,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 300543-05-9P

NAME)

RL: SPN (Synthetic preparation); PREP (Preparation) (bispidine-derived N-acyliminium ions in stereocontrolled construction of the BCD rings of sparteine synthesis) 300543-05-9 CAPLUS

RN CN3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 2-(2-propenyl)-, 3-(1,1-dimethylethyl) 7-ethyl ester, (1R,2S,5S)-rel- (9CI) (CA INDEX

Relative stereochemistry.

RE.CNT

RE

- (1) Beak, P; Acc Chem Res 1996, V29, P552 CAPLUS (2) Bohlmann, F; Chem Ber 1973, V106, P3026 CAPLUS (3) Curtis, M; J Org Chem 1999, V64, P2996 CAPLUS
- (4) Han, G; Angew Chem, Int Ed Engl 2000, V39, P237 CAPLUS
- (5) Han, G; J Org Chem 1996, V61, P9483 CAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 11 OF 97 CAPLUS COPYRIGHT 2001 ACS
AN
     2000:260016 CAPLUS
DN
     132:284247
ΤI
     A dried or frozen pharmaceutical preparation containing a class III
     antiarrhythmic compound
TN
     Bjore, Annika; Granath, Anna-Karin
     Astrazeneca AB, Swed.
PA
     PCT Int. Appl., 31 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                           DATE
                                           APPLICATION NO. DATE
                                           _____
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             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM
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             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     BR 9906869
                            20001017
                                          BR 1999-6869
                                                            19991011
                       Α
     EP 1043997
                            20001018
                                           EP 1999-970322
                       Α1
                                                            19991011
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     NO 2000002986
                            20000609
                                           NO 2000-2986
                                                            20000609
                     Α
PRAI SE 1998-3517
                       Α
                            19981015
     WO 1999-SE1828
                            19991011
                       W
OS
     MARPAT 132:284247
AΒ
     The present invention relates to dried prepns. contg. a class III
     antiarrythmic compd. in the form of cryst. or amorphous salt or any
     combination thereof, where the counterion is selected from
     pharmaceutically acceptable water-sol. org. or inorg. acids. The present
     invention also relates to frozen prepns. contg. a class III antiarrhythmic
     compd. in the form of salt soln., where the counterion is selected from
     pharmaceutically acceptable water-sol. org. or inorg. acids. Preferred
     prepns. contain a salt of the compd. 3,7-diazabicyclo[3.3.1]-nonane-3-
     carboxylic acid 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-1,1-
     dimethylethyl ester (Compd. A). Further aspects of the present invention
     include salts of Compd. A per se, processes for prepg. the prepn., as well
     as use of the prepns. for prophylaxis and/or treatment of cardiac
     arrhythmia.
IT
     227940-01-4 263892-43-9
     RL: BAC (Biological activity or effector, except adverse); THU
     (Therapeutic use); BIOL (Biological study); USES (Uses)
        (freeze-dried pharmaceuticals contq. antiarrhythmic
        diazabicyclononanecarboxylate deriv.)
     227940-01-4 CAPLUS
RN
CN
     3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2R)-3-(4-
     cyanophenoxy) - 2 - hydroxypropyl] -, 1,1 - dimethylethyl ester (9CI)
                                                                    (CA INDEX
     NAME)
```

Absolute stereochemistry.

RN 263892-43-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2R)-3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 227940-01-4 CMF C22 H31 N3 O4

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6 CDES 1:R2:R*,R*

Absolute stereochemistry.

IT 227940-00-3P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of diazabicyclononanecarboxylate deriv. as antiarrhythmic agent)

RN 227940-00-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 227940-70-7P 227940-71-8P 227940-72-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of diazabicyclononanecarboxylate deriv. as antiarrhythmic agent)

RN 227940-70-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-oxo-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-71-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-72-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 263892-42-8P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of diazabicyclononanecarboxylate deriv. as antiarrhythmic agent)

RN 263892-42-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 227940-00-3 CMF C22 H31 N3 O4

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6 CDES 1:R2:R*,R*

Absolute stereochemistry.

RE.CNT 2

RE

- (1) Astra Aktiebolag; WO 9931100 A1 1999 CAPLUS
- (2) Chugai, S; EP 0236679 A1 1987 CAPLUS

Page 58

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ANSWER 12 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 2000:119501 CAPLUS

DN 132:264736

TI Synthesis of chiral amino alcohols embodying the bispidine framework and their application as ligands in enantioselectively catalyzed additions to C=O and C=C groups

AU Spieler, Jan; Huttenloch, Oliver; Waldmann, Herbert

CS Max-Planck-Institut fur moleculare Physiologie, Dortmund, D-44227, Germany

SO Eur. J. Org. Chem. (2000), (3), 391-399 CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 132:264736

AΒ Two generally applicable routes for the synthesis of chiral amino alcs. embodying the bispidine framework have been developed. In a linear route the bispidine framework is built up successively from chiral primary amines via intermediate formation of a piperidinone and a bispidinone. a convergent route an achiral bispidine is formed first and then the N-substituents are introduced by reaction of the nitrogen bases with chiral electrophiles. In order to det. if the bispidine core and its N-substituents can influence the steric course of enantioselective transformations, bispidine amino alcs. built up by these two routes were investigated as chiral ligands in the enantioselectively catalyzed addn. of diethylzinc to aldehydes and chalcone. In general, tridentate ligands contg. one chiral amino alc. fragment and a second amino substituent without a stereogenic center were more efficient than tetradentate ligands with two amino alc. structural units. With the best ligands the enantioselective addn. of diethylzinc to arom. and aliph. aldehydes proceeded with 83-98% ee and the nickel-catalyzed addn. of diethylzinc to chalcone was achieved with up to 85% ee.

IT **280-74-0P**, 3,7-Diazabicyclo[3.3.1] nonane

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of chiral amino alcs. embodying the bispidine framework and their use as ligands in enantioselective addns.)

RN 280-74-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 43

RE

(1) Anon; FR 2274300 1976 CAPLUS

(2) Anon; DE 2428792 1976 CAPLUS

(4) Birk, C; Tetrahedron 1996, V52, P12745 CAPLUS

(5) Bohlmann, F; Chem Ber 1958, V91, P2157 CAPLUS

(7) Bolm, C; Chem Ber 1992, V125, P1191 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 97 CAPLUS COPYRIGHT 2001 ACS

1999:770373 CAPLUS

132:63833

ΤI Conformational switching of 3,7-diacyl-3,7-diazabicyclo[3.3.1] nonanes by metal binding and by solvent changes

ΑU Palyulin, Vladimir A.; Emets, Sergei V.; Chertkov, Vyacheslav A.; Kasper, Christoph; Schneider, Hans-Jorg

Dep. Chemistry, Moscow State Univ., Moscow, 119899, Russia CS

SO Eur. J. Org. Chem. (1999), (12), 3479-3482 CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH

DTJournal

LΑ English

3,7-Diacyl-3,7-diazabicyclo[3.3.1] nonanes (3,7-diacylbispidines) can AΒ switch from antiparallel to parallel conformations upon addn. of LaCl3 thus serving as models for potential allosteric systems. The solvent effect on the conformational switching was also studied.

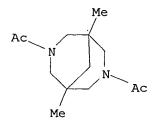
TT 253447-26-6P

> RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC

(conformational switching of 3,7-diacyl-3,7-diazabicyclo[3.3.1]nonanes by metal binding and by solvent changes)

RN 253447-26-6 CAPLUS

3,7-Diazabicyclo[3.3.1]nonane, 3,7-diacetyl-1,5-dimethyl- (9CI) (CA INDEX CN NAME)



RE.CNT

(2) Ashton, P; Chem Eur J 1997, V3, P152 CAPLUS

(4) Baldes, R; Angew Chem Int Ed Engl 1995, V34, P321 CAPLUS

(6) Bauer, H; Chem Ber 1994, V127, P1993 CAPLUS

(7) Feringa, B; Tetrahedron 1993, V49, P8267 CAPLUS(8) Ikeda, T; J Am Chem Soc 1995, V117, P1453 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 14 OF 97 CAPLUS COPYRIGHT 2001 ACS

1999:631969 CAPLUS

DN 132:12427

TI An efficient chemoenzymatic access to chiral 3,7-diazabicyclo[3.3.1]nonane derivatives

AU Danieli, Bruno; Lesma, Giordano; Passarella, Daniele; Silvani, Alessandra; Viviani, Nunzia

CS Dipartimento di Chimica Organica e Industriale, Universita degli Studi di Milano, Centro CNR di Studio per le Sostanze Organiche Naturali, Milan, 21-20133, Italy

SO Tetrahedron (1999), 55(40), 11871-11878 CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

GI

AB Enantiopure 3,7-diazabicyclo[3.3.1]nonane derivs. I and II, potential precursors of quinolizidine alkaloids, were synthesized in high yields, starting from the biocatalytic asymmetrization of .sigma.-sym. 3,5-disubstituted piperidines. Their application to the total synthesis of the new pharmacol. active compds. are also described.

IT 251346-88-0P

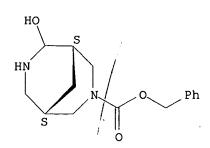
RL: BPN (Biosynthetic preparation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (chemoenzymic access to chiral 3,7-diazabicyclo[3.3.1]nonane derivs.)

RN 251346-88-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 6-hydroxy-, phenylmethyl ester, (1S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





IT 251346-95-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (chemoenzymic access to chiral 3,7-diazabicyclo[3.3.1]nonane derivs.)

RN 251346-95-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 2-hydroxy-, 3-(1,1-dimethylethyl) 7-(phenylmethyl) ester, (1S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

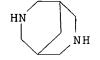
RE.CNT 17

RE

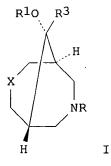
- (3) Danieli, B; J Org Chem 1998, V63, P3492 CAPLUS
- (4) Danieli, B; Tetrahedron 1994, V50, P8837 CAPLUS
- (5) Danieli, B; Tetrahedron: Asymm 1996, V7, P345 CAPLUS
- (6) Dess, D; J Am Chem Soc 1991, V113, P7277 CAPLUS
- (7) Fazylov, S; Zh Obshch Khim 1995, V65, P877 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 15 OF 97 CAPLUS COPYRIGHT 2001 ACS 1999:445821 CAPLUS 131:179515 ΤI Derivatives of 7-aza-3-thiabicyclo[3.3.1] nonanes and 3,7diazabicyclo[3.3.1] nonanes as potential antiarrhythmic agents ΑU Couch, Kevin Michael Oklahoma State Univ., Stillwater, OK, USA CS (1998) 287 pp. Avail.: UMI, Order No. DA9918789 SO From: Diss. Abstr. Int., B 1999, 60(2), 657 DTDissertation English LА AΒ Unavailable IT **280-74-0DP**, 3,7-Diazabicyclo[3.3.1] nonane, derivs. RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. of azathiabicyclononanes and diazabicyclononanes as potential antiarrhythmic agents) RN280-74-0 CAPLUS 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME) CN



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ANSWER 16 OF 97 CAPLUS COPYRIGHT 2001 ACS
AN 
     1999:421688 CAPLUS
     131:58813
DN
ΤI
     Preparation of bicyclic nitrogen compounds as Kv2.1 antagonists
     Bubacz, Dulce Garrido; Dukes, Iain David; McLean, Ed Williams; Noe, Robert
IN
     Anderson; Peat, Andrew James; Szewczyk, Jerzy Ryszard; Thomson, Stephen
     Andrew; Worley, Jennings Franklin, III
PA
     Glaxo Group Limited, UK
SO
     PCT Int. Appl., 53 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
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                            DATE
                                           APPLICATION NO.
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             KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN,
             MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM,
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             TJ, TM
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                       Α1
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             IE, SI, LT, LV, FI, RO
PRAI GB 1997-26630
                       Α
                            19971218
     WO 1998-EP8085
                            19981216
OS
    MARPAT 131:58813
GΙ
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Treatment of non-insulin dependent diabetes mellitus, i.e., administration of antagonists I [R = alkyl, alkenyl, alkoxyalkyl, etc.; R1 = substituted benzyl, substituted benzoyl, etc.; X = S, O, NR2; R3 = H, alkyl] of the delayed rectifier potassium channel Kv2.1, is reported. E.g., anti-3-(4-(3,4-methylenedioxyphenyl)butyl)-7-methyl-3,7-diazabicyclononan-9-ol 4-chlorobenzoate was prepd.

IT 228270-24-4P 228270-26-6P 228270-27-7P

228270-24-4P 228270-26-6P 228270-27-7P 228270-29-9P 228270-30-2P 228270-31-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of bicyclic nitrogen compds. as Kv2.1 antagonists)
RN 228270-24-4 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-(benzoyloxy)-9

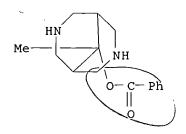
3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-(benzoyloxy)-9-methyl-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

RN 228270-26-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 9-methyl-, benzoate (ester), bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 228270-25-5 CMF C15 H20 N2 O2



CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 228270-27-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(1,3-benzodioxol-5-yl)butyl]-9-(benzoyloxy)-9-methyl-, phenylmethyl ester, (9-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 228270-29-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-hydroxy-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

0 t-Bu0-C N C-OBu-t

RN 228270-30-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-[(4-chlorobenzoyl)oxy]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

RN 228270-31-3 CAPLUS

CN Benzoic acid, 4-chloro-, 3,7-diazabicyclo[3.3.1]non-9-yl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RE.CNT 7

RE

- (2) Izquierdo, M; Journal of Molecular Structure 1989, V213, P175 CAPLUS
- (3) Merck; WO 9716438 A 1997 CAPLUS
- (4) Neurosearch; EP 0528749 A 1993 CAPLUS
- (5) Richter, G; GB 2102801 A 1981 CAPLUS
- (6) Richter, G; WO 9622096 A 1996 CAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 17 OF 97 CAPLUS COPYRIGHT 2001 ACS
     1999:404964 CAPLUS
AN
DN
     131:58860
     Preparation of 3,7-diazabicyclo[3.3.1]nonane-3-carboxylates as
TI
     antiarrhythmic agents
     Strandlund, Gert; Alstermark, Christer; Bjore, Annika; Bjorsne, Magnus;
IN
     Frantsi, Marianne; Halvarsson, Torbjorn; Hoffmann, Kurt-Jurgen; Lindstedt,
     Eva-Lotte; Polla, Magnus
     Astra Aktiebolag, Swed.
PA
     PCT Int. Appl., 129 pp.
SO
     CODEN: PIXXD2
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                                           WO 1998-SE2276
PΙ
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                                           NO 2000-3137
                                                             20000616
                       Α
PRAI SE 1997-4709
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                       Α
     WO 1998-SE2276
                       W
                            19981210
OS
    MARPAT 131:58860
GΙ
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$$R^{3}$$
 R^{4}
 R^{2}
 R^{2}
 R^{3}

AB Title compds. [I; R1,R2 = H or alkyl; R1R2 = OCH2CH2O, (CH2)4-5; R3 = CCR10R11AR; A = bond, alkylene, (CH2)nZ, CONR2O, etc.; B = bond, alkylene, NR23(CH2)r, O(CH2)r; R = (un)substituted Ph; R4 = COXR9; R9 = alkyl, (un)substituted phenyl(alkyl), -naphthyl; R10 = H or OH; R11,R2O,R23 = H or alkyl; X = O or S; Z = NR2O, SOO-2, O; n,r = 0-4] were prepd. Thus,

and the second

4-(NC)C6H4OH was condensed with epichlorohydrin and the product aminated by I (R1 = R2 = H, R4 = CO2CMe3)(II; R3 = H) (prepn. given) to give II [R3 = CH2CH(OH)CH2OC6H4(CN)-4]. Data for biol. activity of I were given. IT 227939-98-2P 227939-99-3P 227940-00-3P 227940-01-4P 227940-02-5P 227940-03-6P 227940-05-8P 227940-06-9P 227940-07-0P 227940-08-1P 227940-09-2P 227940-10-5P

227940-11-6P 227940-12-7P 227940-13-8P 227940-14-9P 227940-15-0P 227940-16-1P 227940-17-2P 227940-18-3P 227940-19-4P 227940-20-7P 227940-21-8P 227940-23-0P 227940-24-1P 227940-25-2P 227940-26-3P 227940-27-4P 227940-28-5P 227940-29-6P 227940-30-9P 227940-31-0P 227940-32-1P 227940-33-2P 227940-34-3P 227940-35-4P 227940-36-5P 227940-39-8P 227940-40-1P 227940-41-2P 227940-42-3P 227940-43-4P 227940-44-5P 227940-45-6P 227940-46-7P 227940-47-8P 227940-48-9P 227940-49-0P 227940-50-3P 227940-51-4P 227940-52-5P 227940-53-6P 227940-54-7P 227940-55-8P

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227940-59-2P 227940-60-5P 227940-61-6P 227940-62-7P 227940-63-8P 227940-64-9P

227940-65-0P 227940-66-1P 227940-67-2P 227940-68-3P 227940-69-4P 227955-64-8P

227955-68-2P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3,7-diazabicyclo[3.3.1]nonane-3-carboxylates as antiarrhythmic agents)

RN 227939-98-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2hydroxypropyl]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C} & \text{C} & \text{C} \\ \hline \\ \text{N} & \text{CH}_2\text{-}\text{CH}\text{-}\text{CH}_2\text{-}\text{O} \end{array}$$

RN 227939-99-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C
$$N$$
 OH N — CH_2 — CH_2 — OH_2 —

RN 227940-00-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 227940-01-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2R)-3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 227940-02-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O & O \\ \hline & O & O & O \\ \hline & N & CH_2 - CH - CH_2 - O \\ \hline \end{array}$$

RN 227940-03-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 227940-05-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 227940-06-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 227940-07-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, cyclopentyl ester (9CI) (CA INDEX NAME)

RN 227940-08-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[4-cyano-2-[(cyclopropylamino)carbonyl]phenoxy]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Page 72

RN 227940-09-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[4-cyano-2-[[(1-methylethyl)amino]carbonyl]phenoxy]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-10-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-hydroxy-3-(4-nitrophenoxy)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-Buo-C
$$N$$
 OH N NO2

RN 227940-11-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-aminophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-12-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-hydroxy-3-[4-[(methylsulfonyl)amino]phenoxy]propyl]-, 1,1-dimethylethyl ester (9CI)

(CA INDEX NAME)

$$\begin{array}{c|c} C & O & O & O \\ \parallel & & & \\ N - CH_2 - CH - CH_2 - O & O \\ \end{array}$$

RN 227940-13-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyano-2-methylphenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-14-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(2-amino-4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-15-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[4-cyano-2-[(methylsulfonyl)amino]phenoxy]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-16-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[4-cyano-2-[(ethylamino)carbonyl]amino]phenoxy]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-17-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(2,4-dicyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C N OH CN
$$\sim$$
 CH₂-CH-CH₂-O \sim CN

RN 227940-18-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-oxo-3-(phenylamino)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-19-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-20-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[(4-cyanophenyl)amino]-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-21-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[(4-cyanophenyl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-23-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-(4-cyanophenyl)-2-hydroxyethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

$$i-PrO-C$$
 N
 N
 CH_2-CH
 CN

RN 227940-24-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-(4-cyanophenyl)ethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

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$$\begin{array}{c|c} O & \\ I - PrO - C & \\ \hline N & \\ N - CH_2 - CH_2 \\ \end{array}$$

RN 227940-25-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-[[(phenylmethoxy)carbonyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \circ & \circ \\ \text{t-BuO-C} & & \circ & \circ \\ & & N & \circ & \circ \\ & N &$$

RN 227940-26-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-[[(4-cyanophenyl)methyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C
$$N$$
 N — CH_2 — CH_2 — N

RN 227940-27-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-2,4-dihydroxybutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-Buo-C
$$N$$
 OH OH N CH₂-CH-CH₂-CH

RN 227940-28-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-hydroxybutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-29-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-hydroxybutyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 227940-30-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxy-2-methylpropyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 227940-31-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxy-2-methylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 227940-32-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 2-hydroxy-1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-33-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1-cyano-1-methylethyl ester (9CI) (CA INDEX NAME)

RN 227940-34-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 2-(3,4-dimethoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

RN 227940-35-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 227940-36-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{Ph}-\mathsf{CH}_2-\mathsf{O}-\mathsf{C} & \mathsf{OH} & \mathsf{OH} \\ \mathsf{N} & \mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}_2-\mathsf{O} & \mathsf{CN} \end{array}$$

RN 227940-39-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester, 7-oxide (9CI) (CA INDEX NAME)

t-BuO-C N OH CN
$$N$$
— CH_2 — CH_2 — CH_2 — OH_2 —

RN 227940-40-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, cyclopentyl ester, 7-oxide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{OH} & \text{O} \\ & \text{O} \\ & \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{N} \\ & \text{N} \\ & \text{C} - \text{O} \end{array}$$

RN 227940-41-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)propyl]-, 1,1-dimethylethyl ester, 7-oxide (9CI) (CA INDEX NAME)

RN 227940-42-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[(4-cyanophenyl)amino]propyl]-, 1,1-dimethylethyl ester, 7-oxide (9CI) (CA INDEX NAME)

t-BuO-C
$$N$$
 N (CH₂)₃-NH N

RN 227940-43-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, butyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{N} & \text{OH} & \text{CN} \\ \hline \\ \text{N} & \text{CH}_2-\text{CH}-\text{CH}_2-\text{O} \\ \hline \end{array}$$

RN 227940-44-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 2-chloroethyl ester (9CI) (CA INDEX NAME)

$$\mathsf{C1CH}_2-\mathsf{CH}_2-\mathsf{O}-\mathsf{C}$$

$$\mathsf{N}$$

$$\mathsf{N}-\mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}_2-\mathsf{O}$$

RN 227940-45-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)

oprocession**i g**eraio e

$$H_2C = CH - CH_2 - O - C$$
 $N - CH_2 - CH - CH_2 - O$
 $N - CH_2 - CH - CH_2 - O$

RN 227940-46-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, propyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & O & \\ &$$

RN 227940-47-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{OH} & \text{OH} \\ \hline & \text{O-CH}_2\text{-CH-CH}_2\text{--N} & \text{O} \\ \hline & \text{N-C-O-CH}_2 \end{array}$$

RN 227940-48-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 4-fluorophenyl ester (9CI) (CA INDEX NAME)

RN 227940-49-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 4-methylphenyl ester (9CI) (CA INDEX NAME)

RN 227940-50-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 4-methoxyphenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{OH} \\ \hline \\ \text{O-CH}_2\text{-CH-CH}_2\text{--N} & \text{O} \\ \hline \\ \text{N--C-O} \end{array}$$

RN 227940-51-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 227940-52-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 227940-53-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)

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RN 227940-54-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[4-(1,1-dimethylethyl)phenoxy]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C N OH N---
$$CH_2-CH-CH_2-O$$

RN 227940-55-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(2-hydroxy-3-phenoxypropyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-56-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-9,9-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-57-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxy-1,1-dimethylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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RN 227940-58-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyano-2-hydroxyphenoxy)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-59-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-2-hydroxybutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C N OH OH
$$N$$
— CH_2 — CH_2 — CH_2 — CH_2

RN 227940-60-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenoxy)-2-hydroxybutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C
$$N$$
 N CH_2 CH_2 CH_2 CH_2 OH_2 OH_3 OH_4 OH_4 OH_5 OH_5 OH_5 OH_6 OH_6

RN 227940-61-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-[(4-cyanophenyl)thio]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-62-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenoxy)-2-butenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C N N—
$$CH_2-CH$$
 $CH-CH_2-O$

RN 227940-63-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-[2-(4-cyanophenoxy)ethoxy]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-64-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C N N— (CH₂)
$$_4$$

RN 227940-65-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[2-(4-cyanophenoxy)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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RN 227940-66-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl ester (9CI) (CA INDEX NAME)

RN 227940-67-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2S)-3-(4-cyanophenoxy)-2-hydroxypropyl]-, cyclopropylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 227940-68-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-, 2-(4-acetyl-1-piperazinyl)ethyl ester (9CI) (CA INDEX NAME)

RN 227940-69-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-

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hydroxy-2-(hydroxymethyl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-Buo-C
$$N$$
 N CH_2 CH_2 OH CN OH

RN 227955-64-8 CAPLUS

CN 7-Aza-3-azoniabicyclo[3.3.1]nonane, 3-[(2R)-3-(4-cyanophenoxy)-2-hydroxypropyl]-7-[(1,1-dimethylethoxy)carbonyl]-3-methyl-, rel-, acetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 227955-63-7 CMF C23 H34 N3 O4

Absolute stereochemistry.

CM 2

CRN 71-50-1 CMF C2 H3 O2

RN 227955-68-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[(2R)-3-(4-cyanophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester, 7-oxide, rel-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 227941-21-1

RL: RCT (Reactant)

(prepn. of 3,7-diazabicyclo[3.3.1]nonane-3-carboxylates as

antiarrhythmic agents)

RN 227941-21-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid (9CI) (CA INDEX NAME)

69407-32-5P 120466-46-8P 227940-70-7P 227940-71-8P 227940-72-9P 227940-73-0P 227940-74-1P 227940-75-2P 227940-76-3P 227940-78-5P 227940-79-6P 227940-80-9P 227940-84-3P 227940-88-7P 227940-90-1P 227940-94-5P 227940-95-6P 227940-96-7P 227940-97-8P 227940-98-9P 227940-99-0P 227941-06-2P 227941-07-3P 227941-17-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of 3,7-diazabicyclo[3.3.1]nonane-3-carboxylates as antiarrhythmic agents) RN69407-32-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{HN} \\ \text{N} \\ \text{CH}_2 - \text{Ph} \end{array}$$

RN120466-46-8 CAPLUS

3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl-3-(phenylmethyl)- (9CI) CN INDEX NAME)

09/623,726

$$Me$$
 N
 CH_2-Ph
 Me

RN 227940-70-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-oxo-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-71-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ph-CH}_2 \\ \hline \\ N \\ \hline \\ N \\ \hline \\ C \\ C \\ O \\ \text{Bu-t} \end{array}$$

RN 227940-72-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-73-0 CAPLUS

CN Benzonitrile, 4-[3-(3,7-diazabicyclo[3.3.1]non-3-yl)-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

RN 227940-74-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 227940-75-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 227940-76-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-78-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyanophenoxy)-2-hydroxypropyl]-9-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 227940-79-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 1,1-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 227940-80-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 1,1-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 227940-84-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[3-(4-cyano-2-nitrophenoxy)-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

t-BuO-C N OH OH NO2
$$\sim$$
 CN NO2

RN 227940-88-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(2-aminoethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-90-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(acetyloxy)-4-(4-cyanophenyl)-2-hydroxybutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C & O & O \\ \hline \\ C & O \\ N & O \\ N & C \\ H_2 - C \\ C \\$$

RN 227940-94-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-[4-(4-cyanophenyl)-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-95-6 CAPLUS

CN Benzonitrile, 4-[4-(3,7-diazabicyclo[3.3.1]non-3-yl)-1-hydroxybutyl]-(9CI) (CA INDEX NAME)

RN 227940-96-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 2-ethoxy-1,1-dimethyl-2-oxoethyl ester (9CI) (CA INDEX NAME)

09/623,726

RN 227940-97-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 2-hydroxy-1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227940-98-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 7-(phenylmethyl)-, 2-(3,4-dimethoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

RN 227940-99-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 2-(3,4-dimethoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

RN 227941-06-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9,9-dimethyl-7-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

09/623,726

RN 227941-07-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9,9-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 227941-17-5 CAPLUS

CN Benzonitrile, 4-[(2S)-3-(3,7-diazabicyclo[3.3.1]non-3-yl)-2-hydroxypropoxy]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●2 HCl

RE.CNT 3

RE

- (1) Basf Aktiengesellschaft; EP 0308843 A2 1989 CAPLUS
- (2) Kall-Chemie Pharma Gmbh; EP 0306871 A2 1989 CAPLUS
- (3) The Board Of Regents Of Oklahoma State University; WO 9107405 A1 1991 CAPLUS

LN3 ANSWER 18 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1999:205876 CAPLUS

DN 130:311780

TI Syntheses and conversion of polyhedral, compounds. 26. Synthesis of new heteropolyhedral compounds by heterocyclization of certain 3,7-disubstituted derivatives of 3,7-diaza- and 1,3,7-triazabicyclo[3.3.1]nonanes

AU Agadzhanyan, Ts. E.; Arutyunyan, G. L.; Movsesyan, R. A.

CS A. L. Mndzhoyan Institute of Fine Organic Chemistry, National Academy of Sciences of the Republic of Armenia, Yerevan, 375014, Armenia

SO Chem. Heterocycl. Compd. (N. Y.) (1999), Volume Date 1998, 34(8), 979-982 CODEN: CHCCAL; ISSN: 0009-3122

PB Consultants Bureau

DT Journal

LA English

OS CASREACT 130:311780

AB The following heterocyclization reactions have been carried out: heterocyclization of 3,7-diacryloyl-3,7-diazabicyclo[3.3.1]nonane by benzylamine, heterocyclization of 3,7-diacryloyl-3,7-bis(.beta.-bromopropionyl)-, and 3,7-bis(.beta.-chloroethyl)-3,7-diazabicyclo[3.3.1]nonanes by hydrogen sulfide, and heterocyclization of 3,7-bis(bromoacetyl)- and 3,7-diacryloyl-1,3, 7-triazabicyclo[3.3.1]nonanes by benzylamine and hydrogen sulfide. New compds. were obtained, based on previously unknown thiadiaza-, triaza-, and tetraazatricyclic systems.

IT 80808-88-4 80808-89-5

RL: RCT (Reactant)

(prepn. of heteropolyhedral compds. by heterocyclization of diaza- and triazabicyclononanes)

RN 80808-88-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(3-bromo-1-oxopropy1)-1,5-dimethyl- (9CI) (CA INDEX NAME)

RN 80808-89-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3,7-bis(1-oxo-2-propenyl)-(9CI) (CA INDEX NAME)

$$H_2C = CH - C$$
 N
 $C - CH = CH_2$
 Me
 Me

RE.CNT 6

RE

- (1) Agadzhanyan, T; Arm Khim Zh 1981, V34, P963 CAPLUS(2) Agadzhanyan, T; Arm Khim Zh 1983, V36, P730 CAPLUS
- (3) Agadzhanyan, T; Chemotherapy of Tumors in the USSR [in Russian] 1982, 35,
- (4) Agadzhanyan, T; Khim Geterotsikl Soedin 1994, 3, P393
- (5) Agadzhanyan, T; Khim Geterotsikl Soedin 1997, 11, P1490
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

M3 ANSWER 19

ANSWER 19 OF 97 CAPLUS COPYRIGHT 2001 ACS

1998:487604 CAPLUS

129:188934

TI Molecular structure of 3-benzyl-1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-one

AU Karapetyan, A. A.; Arutyunyan, A. D.; Agadjanyan, Ts. E.

CS Molecular Structure Research Center, Armenian Academy of Sciences, Armenia

SO J. Struct. Chem. (1998), 39(1), 143-146 CODEN: JSTCAM; ISSN: 0022-4766

PB Consultants Bureau

DT Journal

LA English

AB The crystal and mol. structures of the title compd. were detd. by x-ray crystallog. A double-chair conformation was confirmed.

crystallog. A double-chair conformation was confirmed.

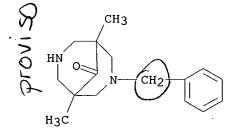
IT 107606-88-2, 3,7-Diazabicyclo[3.3.1]nonan-9-one,
1,5-dimethyl-3-(phenylmethyl)-

RL: PRP (Properties)

(crystal and mol. structure and conformation of benzyldimethyldiazabicyclononanone)

RN 107606-88-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



09/623,726

L18 ANSWER 20 OF 97 CAPLUS COPYRIGHT 2001 ACS

1998:484412 CAPLUS

129:189250

TI Synthesis and conversions of polyhedral compounds. 25. Synthesis and conversions of certain oxindole derivatives of 1,3-diazaadamantane and 3,7-diazabicyclo[3.3.1]nonane

AU Agadzhanyan, Ts. E.; Gevorkyan, K. A.

CS A. L. Mndzhoyan Institute of Fine Organic Chemistry, Academy of Sciences of the Republic of Armenia, Yerevan, 375014, Armenia

SO Chem. Heterocycl. Compd. (N. Y.) (1998), Volume Date 1997, 33(11), 1288-1291

CODEN: CHCCAL; ISSN: 0009-3122

PB Consultants Bureau

DT Journal

LA English

AB By the reaction of 1,5-dimethyl-9-oxo-3,7-diazabicyclo[3.3.1]nonane with isatin and a no. of its derivs., spiro(1,3-diazaadamantane-2,3'-oxindoles) have been synthesized. In the case of 5-bromoisatin, either 3-(3-hydroxyoxindolyl)-3,7-diazabicyclo[3.3.1]nonane or the corresponding spirane is obtained, depending on the temp. The interaction of these products with acetic anhydride has been studied.

IT 80808-96-4

RL: RCT (Reactant)

(reactions of diazabicyclononane with isatins)

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)

IT 147698-79-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (reactions of diazabicyclononane with isatins)

RN 147698-79-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-diacetyl-1,5-dimethyl- (9CI) (CA INDEX NAME)

ANSWER 21 OF 97 CAPLUS COPYRIGHT 2001 ACS 1998:314847 CAPLUS DN 129:42327 ΤI Linked streptocyanine colorants IN Kato, Takashi; Okazaki, Renji PA Fuji Photo Film Co., Ltd., Japan so Jpn. Kokai Tokkyo Koho, 5 pp. CODEN: JKXXAF DTPatent LΑ Japanese FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE _____ ____ ~----_____ PΙ JP 10130516 19980519 Α2 JP 1996-286272 19961029

AB Two streptocyanine compds. are linked to show absorption being shifted in a region of shorter wavelength. Thus, 0.14 g N-(2,4dinitrophenyl)pyridinium chloride was treated with 65 mg bispidine in MeOH/H2O and further treated with NaClO4 to give 23 mg bisstreptocyanine having .lambda.max 370 nm (.vepsiln. = 2.08 .times. 105; MeOH).

IT280-74-0, Bispidine RL: RCT (Reactant)

> (manuf. of bisstreptocyanine colorants having absorption at shorter wavelength)

280-74-0 CAPLUS RN

CN 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)



09/623,726

LTS ANSWER 22 OF 97 CAPLUS COPYRIGHT 2001 ACS

1998:53390 CAPLUS

DN 128:180115

TI Stereochemistry of N-acetyl-r-2,c-4-diphenyl-3-azabicyclo[3.3.1]nonanes and N-ethoxycarbonyl-r-2,c-4-diphenyl-3-azabicyclo[3.3.1]nonane

AU Jeyaraman, R.; Ponnuswamy, S.

CS Department of Chemistry, Bharathidasan University, Tiruchirapalli, 620 024, India

SO Indian J. Chem., Sect. B: Org. Chem. Incl. Med. Chem. (1997), 36B(9), 730-737

CODEN: IJSBDB; ISSN: 0376-4699

PB National Institute of Science Communication, CSIR

DT Journal

LA English

GI.

AB The conformational preferences of N-acetyl-r-2,c-4-diphenyl-3-azabicyclo[3.3.1] nonane I and N-ethoxycarbonyl-and N-acetyl-r-2,c-4,t-6,t-8-tetraphenyl-3,7-diazabicyclo[3.3.1] nonanes II (R= CO2Et,COMe) have been studied using NMR spectral techniques. The azabicyclo[3.3.1] nonane I is found to prefer a twin-chair conformation with a slight flattening at the nitrogen end. In the case of diazabicycles II both the ethoxycarbonylation and acetylation reactions are found to take place only at the boat end of the parent amine and the preferred conformation of the products is found to be twin-chair with flattening at C1-C2-N3-C4-C5 part of the ring in both cases. The energy barrier for the N-CO rotation in N-ethoxycarbonyl deriv. 6 has been detd. from the dynamic 1H NMR studies and the barrier for N- CO rotation is found to be 50.8 kJ mol-1, much less than that of N-nitroso analogs.

IT 203190-52-7P, N-(Ethoxycarbonyl)-r-2, c-4-diphenyl-3-

azabicyclo[3.3.1]nonane 203190-53-8P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(dynamic NMR conformational anal. of ethoxycarbonyl-and acetyltetraphenyldiazabicyclononanes)

RN 203190-52-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 2,4,6,8-tetraphenyl-, ethyl ester, (2R,4S,6S,8R)-rel-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN203190-53-8 CAPLUS CN3,7-Diazabicyclo[3.3.1]nonane, 3-acetyl-2,4,6,8-tetraphenyl-, (2R, 4S, 6S, 8R) -rel-[partial] - (9CI) (CA INDEX NAME)

Relative stereochemistry.

ΙT 75541-42-3

RL: RCT (Reactant)

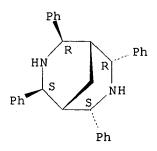
(starting material; prepn. of ethoxycarbonyldiphenylazabicyclononane)

RN75541-42-3 CAPLUS

3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetraphenyl-, (2-endo,4-endo,6-CN

exo, 8-exo) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



11/3

ANSWER 23 OF 97 CAPLUS COPYRIGHT 2001 ACS

1997:597560 CAPLUS

127:308422

TI Linear and Stack Oligostreptocyanines. Effects of Relative Orientation of Chromophores on Redox Potentials of Dye Aggregates

AU Katoh, Takashi; Inagaki, Yoshio; Okazaki, Renji

CS Fuji Photo Film Co., Ltd., 210 Nakanuma, Minami-ashigara, Kanagawa, 250-01, Japan

SO Bull. Chem. Soc. Jpn. (1997), 70(9), 2279-2286 CODEN: BCSJA8; ISSN: 0009-2673

PB Chemical Society of Japan

DT Journal

LA English

AB Linear and stack pentamethinestreptocyanine oligomers were prepd. in which streptocyanines are covalently connected to each other. The absorption bands of the linear oligomers showed bathochromic shifts compared to that of the corresponding monomer, while the absorption band of the stack dimer was hypsochromically shifted. These spectral shifts were reproduced by a calcn. with the INDO/S-CI method and are in agreement with those based upon a mol. exciton theory. The redox potentials of the linear oligomers underwent a pos. shift due to the Coulombic interaction compared to those of the streptocyanine monomer. The pos. shift of the redn. potential and the neg. shift of the oxidn. potential of the stack dimer are explained in terms of the Coulombic and orbital interactions.

IT **280-74-0**, Bispidine

RL: RCT (Reactant)

(synthesis of stack dimer; effects of relative chromophore orientation on redox potentials of linear and stack streptocyanine dye dimers and trimers)

RN 280-74-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)



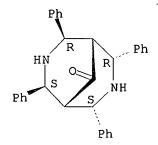
Page 103

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09/623,726
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ANSWER 24 OF 97 CAPLUS COPYRIGHT 2001 ACS 1997:491283 CAPLUS 127:81001 DN ΤI Conformation and Stereodynamics of N, N'-Dinitroso-2, 4, 6, 8-tetraaryl-3, 7diazabicyclo[3.3.1] nonanes AU Gdaniec, Maria; Pham, Marzena; Polonski, Tadeusz Faculty of Chemistry, A. Mickiewicz University, Poznan, 60-780, Pol. CS J. Org. Chem. (1997), 62(16), 5619-5622 SO CODEN: JOCEAH; ISSN: 0022-3263 PB American Chemical Society DT Journal LΑ English OS CASREACT 127:81001 AΒ The mol. mechanics calcns., X-ray crystallog., and 1H NMR consistently have shown that N,N'-dinitrosation of 2,4,6,8-tetraaryl-3,7diazabicyclo[3.3.1] nonanes changes their conformation from a chair-boat to a twin-chain one with two aryl groups occupying axial positions and remaining two equatorial ones. The strong allylic A(1,3) strain, caused by interaction of the NNO group with the neighboring equatorial aryl substituents, leads to a pyramidalization of the amino nitrogen and a significant deviation of the corresponding nitrosamine group from planarity, whereas the second nitrosamine group remains essentially planar. The variable temp. NMR measurements have revealed two different barriers to the N-N rotation in the title compds. 65732-77-6 75541-42-3 75549-52-9 191345-76-3 RL: RCT (Reactant) (conformation and stereodynamics of N,N'-dinitroso-2,4,6,8-tetraaryl-3,7-diazabicyclo[3.3.1]nonanes)

Relative stereochemistry.

65732-77-6 CAPLUS



RN

CN

RN 75541-42-3 CAPLUS 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetraphenyl-, (2-endo,4-endo,6-CN exo, 8-exo) - (9CI) (CA INDEX NAME)

3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl-,

(2R, 4S, 6S, 8R) - rel - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 75549-52-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methylphenyl)-, (2R,4S,6S,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 191345-76-3 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-fluorophenyl)-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

A ANSWER 25 OF 97 CAPLUS COPYRIGHT 2001 ACS

1997:172468 CAPLUS

DN 126:199654

TI (.pi.-Allyl)palladium Complexes with N,N'-Diphenylbispidinone Derivatives as a New Type of Chelating Nitrogen Ligand: Complexation Studies, Spectroscopic Properties, and an X-ray Structure of (3,7-Diphenyl-1,5-dimethylbispidinone)[(1,3-.eta.3-propenyl)-palladium]
Trifluoromethanesulfonate

AU Gogoll, Adolf; Grennberg, Helena; Axen, Andreas

CS Department of Organic Chemistry, University of Uppsala, Uppsala, 751 21, Swed.

SO Organometallics (1997), 16(6), 1167-1178 CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society

DT Journal

LA English

OS CASREACT 126:199654

AB A series of 3,7-diazabicyclo[3.3.1] nonane (bispidine) derivs. have been synthesized, and their properties as bidentate nitrogen ligands for (.pi.-allyl)palladium complexes have been investigated. Complexes of these ligands and of N,N'-diphenylpiperazine and N,N'-diphenyl-1,4diazacyclooctane with (1,3-.eta.3-propenyl)palladium are described, in particular their effects on the proton chem. shifts of the .pi.-allyl ligand. Ligand dynamics of the complexes is discussed. The structure of [(3,7-diphenyl-1,5-dimethylbispidinone)(1,3-.eta.3-propenyl)Pd]CF3SO3 has been detd. by x-ray crystallog. N,N'-Diphenylbispidine derivs. show an unusually large steric interaction with the .pi.-allyl ligand, indicated by a tilt of the .pi.-allyl plane toward the N-Pd-N plane by 122.8(8).degree. Chem. shift changes of the .pi.-allyl protons due to the arom. ring current are related to the geometry of the complexes. The ligands are tested on the larger 2-methylene-6,6dimethylbicyclo[3.1.1]hept-2,3,10-.eta.3-enyl ligand, demonstrating their potential as chem. shift reagents.

IT 80808-96-4P

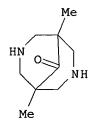
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of allylpalladium complexes with diphenylbispidinone derivs. as new type of chelating nitrogen ligand and their complexation studies and spectroscopic properties)

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)

1996年1996年 新安徽安徽安徽



3 ANSWER 26 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1997:135687 CAPLUS

DN 126:219919

TI The design of a new type of very rigid tetradentate ligand

AU Comba, Peter; Nuber, Bernhard; Ramlow, Anne

CS Anorg.-Chem. Inst. Univ., Heidelberg, 69120, Germany

SO J. Chem. Soc., Dalton Trans. (1997), (3), 347-352

CODEN: JCDTBI; ISSN: 0300-9246

PB Royal Society of Chemistry

DT Journal

LA English

AB Mol. mechanics calcns. were used to compute the structural properties of a new type of very rigid tetradentate ligand for tetrahedral coordination geometries. The calcns. indicate that the pendant arms of the disubstituted bispidine (3,7-diazabicyclo[3.3.1]nonane) backbone need to form six-membered chelate rings with the metal to allow a distorted tetrahedral geometry. Smaller rings lead to five-(trigonal bipyramidal) or six-coordinate (octahedral) transition-metal compds. The quality of these predictions is supported by the exptl. detd. structure of a Co(II) compd. of the ligand with coordinated pyridine substituents (five-membered chelate rings) and an addnl. bidentate nitrate ligand. Comparison of the computed structures with the crystal structure of the Co(II) compd. and with that of a ligand with Me-protected Ph substituents supports the rigidity of the bispidine backbone and indicates that rotation of coordinating side chains around a C-C single bond is the only flexibility in these ligands.

IT 280-74-0D, 3,7-Diazabicyclo[3.3.1]nonane, derivs. with pendant arms, cobalt complexes

RL: PRP (Properties)

(mol. mechanics calcns. of structural properties of very rigid tetradentate ligand in cobalt complex)

RN 280-74-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)



🔀 ANSWER 27 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN - 1997:57952 CAPLUS

DN 126:185747

TI Chemical shift assignment of geminal protons in 3,7-diazabicyclo[3.3.1]nonanes: an unexpected deviation from the axial/equatorial chemical shift order

AU Gogoll, Adolf; Grennberg, Helena; Axen, Andreas

CS Department of Organic Chemistry, University of Uppsala, Uppsala, 751 21, Swed.

SO Magn. Reson. Chem. (1997), 35(1), 13-20 CODEN: MRCHEG; ISSN: 0749-1581

PB Wiley

DT Journal

LA English

AB The chem. shift order of axial and equatorial methylene protons in 1,5-disubstituted 3,7-diazabicyclo [3.3.1] nonan-9-ones may be altered by substituents in the 1,5-positions, but the corresponding alcs. behave differently. Unambiguous signal assignments for a series of the title compds. are provided, based on 3JCH coupling consts. and on {1H} 13C heteronuclear Overhauser effects. Substituent anisotropy effects as a source of the chem. shift changes are discussed.

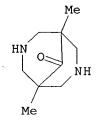
IT 80808-96-4

RL: PRP (Properties)

(deviation from axial/equatorial chem. shift order and chem. shift assignment of geminal protons in 3,7-diazabicyclo[3.3.1]nonanes)

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)



09/62/,726

ANSWER 28 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN > 1996:411968 CAPLUS

DN 125:104282

TI Search for the pharmacophore in kappa-agonistic diazabicyclo[3.3.1]nonan-9-one-1,5-diesters and arylacetamides

AU Brandt, Wolfgang; Drosihn, Susanne; Haurand, Michael; Holzgrabe, Ulrike; Nachtsheim, Corina

CS Pharm. Inst., Univ. bonn, Bonn, 53115, Germany

SO Arch. Pharm. (Weinheim, Ger.) (1996), 329(6), 311-323 CODEN: ARPMAS; ISSN: 0365-6233

DT Journal

LA English

AΒ Several heterocyclic bicyclo[3.3.1]nonan-9-ones were found to have a high affinity to .kappa. opioid receptors. 3,7-Diazabicyclononanones with 2,4-dipyridyl side chains were the most potent agonists whereas the corresponding 3-oxa-7-azabicyclo[3.3.1]nonan-9-one and compds. with Ph substituents in 2 and 4 position are almost inactive. The purpose of this study was to unravel the active conformation of the bicyclononanones using well-known .kappa.-selective agonists such as ketocyclacocine, arylacetamides, several isoquinolines, CI-977, and four stereoisomers of EMD-61753 for comparison. In order to det. the geometry of the diazabicycles in soln. pH-dependent NMR measurements of the bicycles were recorded and the results were related to the geometries of the aforementioned .kappa. agonists obtained from semiempirical PM3 calcns. A chair-boat conformation and a protonation at the N7 nitrogen atom of the diazabicyclononanones were found to be the pharmacophoric conformation. Comparison of the spatial arrangements, electrostatic, hydrophobic, and hydrogen bonding potentials of all .kappa.-selective agonists led to a model of structure-activity relationships of ligands of the .kappa. receptor. The arrangement of the pharmacophoric elements is characterized by an almost parallel orientation of a carbonyl and a protonated NH function in conjunction with at least one arom. ring. Ketocyclazocine is only able to adopt this parallel orientation when the nitrogen is inverted relative to the x-ray structure. Furthermore, two binding sites for the arom. rings are discussed. The pharmacol. results of all considered bicyclononanone derivs. as well as of the four enantiomers of EMD-61753 can be understood and consistently explained in this way.

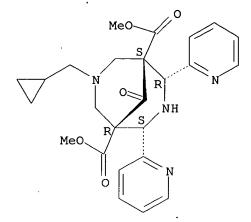
IT 124189-56-6

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmacophore in .kappa.-agonistic diazabicyclo[3.3.1]nonan-9-one-1,5-diesters and arylacetamides)

RN 124189-56-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-(cyclopropylmethyl)-9-oxo-2,4-di-2-pyridinyl-, dimethyl ester, (endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



JAS

DN

ANSWER 29 OF 97 CAPLUS COPYRIGHT 2001 ACS

1996:326442 CAPLUS

125:86610

Novel 3,7-Diheterabicyclo[3.3.1]nonanes That Possess Predominant Class III Antiarrhythmic Activity in 1-4 Day Post Infarction Dog Models: X-ray Diffraction Analysis of 3-[4-(1H-Imidazol-1-yl)benzoyl]-7-isopropyl-3,7-diazabicyclo[3.3.1]nonane Dihydroperchlorate

AU Garrison, Gregory L.; Berlin, K. Darrell; Scherlag, Benjamin J.; Lazzara, Ralph; Patterson, Eugene; Fazekas, Tamas; Sangiah, Subbiah; Chen, Chun-Lin; Schubot, F. D.; van der Helm, Dick

CS Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078, USA

SO J. Med. Chem. (1996), 39(13), 2559-2570 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

GΙ

AΒ Several 3,7-diheterabicyclo[3.3.1] nonanes were prepd. and screened in the Harris dog model for their ability to abolish pace-induced and sustained ventricular tachycardia (SVT) or prevent induction of ventricular tachycardia. In addn., an electrophysiol. examn. was made in the infarcted hearts of each animal to det. if more than one class activity was present. The examples exhibited predominately class III antiarrhythmic activity via a prolongation of the ventricular effective refractory period (VERP) in the models, although there may well be an underlying class Ib action present as exemplified by the ability of several of the agents to slow conduction in the myocardial infarcted dog hearts. 3-[4-(1H-Imidazol-1-yl)benzoyl]-7-isopropyl-3,7diazabicyclo[3.3.1] nonane dihydroperchlorate (I) displayed powerful class III activity in the model systems while several other 3,7diheterabicyclo[3.3.1] nonanes exhibited various degrees of class III action. An X-ray diffraction anal. revealed that this compd. had a 3,7-diazabicyclo[3.3.1] nonane bicyclic unit in a chair-chair conformation. IT 129039-76-5

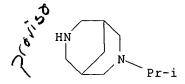
RL: RCT (Reactant)

。如此**的是我们的**

(prepn. and antiarrythmic activity of 3,7-diazabicyclo[3.3.1]nonanes) 129039-76-5 CAPLUS

RN

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-methylethyl)- (9CI) (CA INDEX NAME)

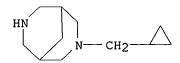


IT 173973-38-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and antiarrythmic activity of 3,7-diazabicyclo[3.3.1]nonanes)

RN 173973-38-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(cyclopropylmethyl)- (9CI) (CA INDEX NAME)



AS ANSWER 30 OF 97 CAPLUS COPYRIGHT 2001 ACS

N 1995:1006741 CAPLUS

DN 124:176165

TI N-alkyl and N-acyl derivatives of 3,7-diazabicyclo[3.3.1] nonanes and selected salts thereof as multi-class antiarrhythmic agents

IN Berlin, Kenneth D.; Garrison, Gregory L.; Sangiah, Subbiah; Clarke, Cyril R.; Chen, Chun Lin; Lazzara, Ralph; Scherlag, Benjamin J.; Patterson, Eugene S.; Burrows, George E.

PA Oklahoma State University, USA

SO U.S., 20 pp.

CODEN: USXXAM

DT Patent

LA English

FAN CNT 1

FAN. CNT I									
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
ΡI	US 5468858	Α	19951121	US 1993-144639	19931028				
	US 5786481	Α	19980728	US 1995-545341	19951019				
PRAI	US 1993-144639		19931028						
os	MARPAT 124:17616								
GT									

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{N} \end{array} \begin{array}{c} \text{N} \\ \text{N} \\ \text{N} \end{array}$$

AB A variety of 3,7-diazabicyclo[3.3.1] nonanes and selected derivs. are disclosed as multi-class antiarrhythmic agents and intermediates thereof. Claimed compds. include I [Q = RN where R = iso-Pr or cyclopropylmethyl; Z = CH2; Y = ArCON where Ar = (un) substituted aryl] and their hydrochloride, hydroperchlorate, fumarate, and other salts. For example, 3-isopropyl-3,7-diazabicyclo[3.3.1] nonane underwent N-acylation with 4-FC6H4COCl, and the product fluoride was condensed with imidazole in the presence of K2CO3 and 18-crown-6, to give title compd. II, isolated as the dihydroperchlorate. At 3-6 mg/kg in dogs with myocardial infarctions and induced ventricular tachycardia, II increased ventricular effective refractory period, prolonged QT by 30%, lowered heart rate by 20-40 beats/min, and prevented sustained ventricular tachycardia (Class I and III activity).

IT 173973-46-1P

RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-alkyl and N-acyl diazabicyclononane derivs. as multi-class antiarrhythmics)

RN 173973-46-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-methylethyl)-7-[(4-nitrophenyl)acetyl]-

્રા ત્વારો કરો છે. આ ત્વારો કરો કરો કરો છે.

(9CI) (CA INDEX NAME)

IT 173973-47-2P 173973-48-3P 173973-49-4P 173973-50-7P 173973-51-8P 173973-52-9P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-alkyl and N-acyl diazabicyclononane derivs. as multi-class antiarrhythmics)

RN 173973-47-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-methylethyl)-7-[(4-nitrophenyl)acetyl]-, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 173973-46-1 CMF C18 H25 N3 O3

CM 2

CRN 7601-90-3 CMF Cl H O4

RN 173973-48-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-[(4-aminophenyl)acetyl]-7-(1-methylethyl)-(9CI) (CA INDEX NAME)

RN 173973-49-4 CAPLUS

Page 115

三烷 编成本的 資色語

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-methylethyl)-7-[[4-[(methylsulfonyl)amino]phenyl]acetyl]- (9CI) (CA INDEX NAME)

RN 173973-50-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-methylethyl)-7-[[4[(methylsulfonyl)amino]phenyl]acetyl]-, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 173973-49-4 CMF C19 H29 N3 O3 S

CM 2

CRN 7601-90-3 CMF Cl H O4

RN 173973-51-8 CAPLUS

CN Acetamide, N-[4-[2-[7-(1-methylethyl)-3,7-diazabicyclo[3.3.1]non-3-yl]-2-oxoethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 173973-52-9 CAPLUS

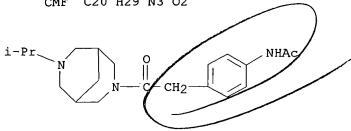
CN Acetamide, N-[4-[2-[7-(1-methylethyl)-3,7-diazabicyclo[3.3.1]non-3-yl]-2-

Page 116

oxoethyl]phenyl]-, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 173973-51-8 CMF C20 H29 N3 O2



CM 2

CRN 7601-90-3 CMF C1 H O4

IT 129039-76-5, 3-Isopropyl-3,7-diazabicyclo[3.3.1]nonane

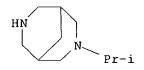
RL: RCT (Reactant)

(starting material; prepn. of N-alkyl and N-acyl diazabicyclononane derivs. as multi-class antiarrhythmics)

RN 129039-76-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1] nonane, 3-(1-methylethyl)- (9CI) (CA INDEX NAME)

Droviso

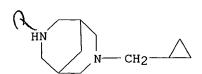


IT 173973-38-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (starting material; prepn. of N-alkyl and N-acyl diazabicyclononane derivs. as multi-class antiarrhythmics)

RN 173973-38-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(cyclopropylmethyl)- (9CI) (CA INDEX NAME)



ANSWER 31 OF 97 CAPLUS COPYRIGHT 2001 ACS

AM - 1995:904877 CAPLUS

DN 124:117427

Synthesis and transformations of polyhedral compounds. 21. Synthesis and antitumor properties of derivatives of 1,3-diaza-2-phosphaadamantane, phosphoryl-containing 3,7-diazabicyclo[3.3.1]nonane, and 1,3-diazaadamantane

AU Arutyunyan, G. L.; Chachoyan, A. A.; Shkulev, V. A.; Adamyan, G. G.; Aqadzhanyan, Ts. E.; Garibdzhanyan, B. T.

CS Inst. Tonkoi Org. Khim., Yerevan, Armenia

SO Khim.-Farm. Zh. (1995), 29(3), 33-5

CODEN: KHFZAN; ISSN: 0023-1134

DT Journal

LA Russian

OS CASREACT 124:117427

GΙ

III

Me

$$\begin{array}{c|c}
Me \\
N-P=0 \\
X & IV
\end{array}$$

II

AB Title compds., e.g., I [X = OPh, N(CH2CH2Cl)2], II, III (same X), and IV (same X) were prepd. from 1,5-dimethyl-9-oxo-3,7-diazabicyclo[3.3.1]nonane and 5,7-dimethyl-6-oxo-1,3-diazaadamantanes and tested for antitumor activity. Derivs. of 1,3-diaza-2-phosphaadamantane are significantly more active than derivs. of 3,7-diazabicyclo[3.3.1]nonane or 1,3-diazaadamantane.

IT 172882-04-1

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(prepn. and antitumor activity of diazaphosphaadamantane derivs. and phosphoryl-contg. derivs. of diazabicyclononane and diazaadamantane) 172882-04-1 CAPLUS

RN 172882-04-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-, dihydrochloride (9CI)
(CA INDEX NAME)

2 HCl

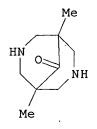
IT 80808-96-4

RL: RCT (Reactant)

(prepn. and antitumor activity of diazaphosphaadamantane derivs. and phosphoryl-contg. derivs. of diazabicyclononane and diazaadamantane)

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)



ANSWER 32 OF 97 CAPLUS COPYRIGHT 2001 ACS 1995:785013 CAPLUS DN 123:188602 ΤI Antiarrhythmic 3-benzoyl-3,7-diazabicyclo[3.3.1]nonanes Schoen, Uwe; Brueckner, Reinhard; Meil, Joerg; Thormaehlen, Dirk IN Kali-Chemie Pharma GmbH, Germany PA SO Eur. Pat. Appl., 11 pp. CODEN: EPXXDW DTPatent German T.A FAN.CNT 1 PATENT NO. DATE APPLICATION NO. KIND DATE -----PΙ EP 665014 **A1** 19950802 EP 1995-100953 19950125 B1 19970903 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE 19950803 DE 1994-4402933 19940201 DE 4402933 **A**1 IL 112344 A1 19970610 IL 1995-112344 19950116 CN 1110556 19951025 CN 1995-101603 19950125 Α AT 157539 19970915 AT 1995-100953 19950125 Ε ES 2108497 Т3 19971216 ES 1995-100953 19950125 HU -70173 A2 19950928 HU 1995-263 19950127 CA 2141367 AA 19950802 CA 1995-2141367 19950130 AU 9511468 19950810 AU 1995-11468 19950130 Α1 ZA 9500698 ZA 1995-698 19950130 A 19960207 NO 9500361 NO 1995-361 Α 19950802 19950131 FI 9500423 FI 1995-423 Α 19950802 19950131 JP 07252152 A2 19951003 JP 1995-14209 19950131 US 5532251 19960702 US 1995~382265 19950201 PRAI DE 1994-4402933 19940201

$$R^{1}N$$
 R^{2} N R^{3} R^{4} R^{5}

MARPAT 123:188602

GΙ

The title compds. (I; R1 = C1-6 alkyl, C4-7 cycloalkylalkyl; R2, R3 = lower alkyl, or R2R3 = C3-6 alkylene; R5 = H, halo, CF3, NO2; R4 = R5, CN, R6SO2; R6 = F, lower alkyl) and their acid addn. salts are useful for treatment of arrhythmia in humans and large mammals. Thus, I [R1 = Bu, R2R3 = (CH2)4, R4 = 4-chloro, R5 = H] (II) (2 .mu.mol/kg i.v.) prolonged the effective refractory time in guinea pigs with exptl. tachycardia by 15% and had a min. oral toxic dose of >300 mg/kg in mice. Tablets were prepd. contg. II-HCl 20, corn starch 30, lactose 55, PVP-25 5, Mg stearate 2, and talc 3 parts. II was prepd. by condensation of 7-butyl-9,9-tetramethylene-3,7-diazabicyclo[3.3.1]nonane with 4-chlorobenzoyl chloride.

IT 120466-42-4 122032-37-5 167553-37-9 167553-42-6

RL: RCT (Reactant)

(antiarrhythmic benzoyldiazabicyclononanes)

RN 120466-42-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9,9-dimethyl- (9CI) (CA INDEX

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NAME)

RN 122032-37-5 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(cyclopropylmethyl)-9,9-dimethyl- (9CI)
(CA INDEX NAME)

$$Me \xrightarrow{HN} N \longrightarrow CH_2 \xrightarrow{N}$$

RN 167553-37-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9-methyl-9-propyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 167553-42-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-hexyl-9,9-dimethyl- (9CI) (CA INDEX NAME)

Me
$$\stackrel{\text{HN}}{\longrightarrow}$$
 $\stackrel{\text{N}}{\longrightarrow}$ (CH₂) 5 - Me

ANSWER 33 OF 97 CAPLUS COPYRIGHT 2001 ACS 1995:785009 CAPLUS ΑN 123:188601 DN. Antiarrhythmic 3-phenylsulfonyl-3,7-diazabicyclo[3.3.1] nonanes ΤI Schoen, Uwe; Farjam, Arman; Brueckner, Reinhard; Ziegler, Dieter IN PA Kali-Chemie Pharma GmbH, Germany SO Eur. Pat. Appl., 20 pp. CODEN: EPXXDW DT Patent LΑ German FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE ΡI EP 665228 19950802 EP 1995-100954 19950125 Α1 EP 665228 В1 19990714 BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, R: AT, DE 4402931 Α1 19950803 DE 1994-4402931 19940201 IL 112364 **A1** 19980104 IL 1995-112364 19950117 CN 1111631 19951115 CN 1995-101498 19950125 Α AT 182149 E 19990715 AT 1995-100954 19950125 ES 2133593 Т3 19990916 ES 1995-100954 19950125 HU 70174 **A**2 19950928 HU 1995-262 19950127 CA 2141366 AA 19950802 CA 1995-2141366 19950130 AU 9511564 A1 19950810 AU 1995-11564 19950130 19960207 ZA 9500697 ZA 1995-697 Α 19950130 PL 1995-307000 PL 180075 В1 20001229 19950130 FI 9500422 Α 19950802 FI 1995-422 19950131 NO 9500360 Α NO 1995-360 19950802 19950131 JP 07267954 A2 19951017 JP 1995-14204 19950131 US 5576327 Α 19961119 US 1995-382262 19950201 US 5635511 Α 19970603 US 1996-594946 19960131 PRAI DE 1994-4402931 19940201 US:1995-382262 Α3 19950201 MARPAT 123:188601 OS GΙ

$$R^{1}N$$
 R^{2} N SO_{2} R^{4} R^{5}

AB The title compds. (I; R1 = C1-6 alkyl, C4-7 cycloalkylalkyl; R2, R3 = lower alkyl, or R2R3 = C3-6 alkylene; R4 = halo, NO2, CF3, CN, alkoxycarbonyl, alkanesulfonamido, carboxamido; R5 = H, halo) are useful for treatment of cardiac arrhythmia in humans and large mammals. Thus, I (R1 = Bu, R2 = R3 = Me, R4 = 4-CN, R5 = H) (II) (1 .mu.mol/kg i.v.) prolonged the effective refractory time by 15% in guinea pigs with exptl. tachycardia, and had a min. oral toxic dose >300 mg/kg in mice. II-HCl was prepd. by condensation of 7-butyl-9,9-dimethyl-3,7-diazabicyclo[3.3.1]nonane with 4-cyanobenzenesulfonyl chloride. Tablets were prepd. contg. II-HCl 20, corn starch 69, lactose 135, gelatin (as 10% soln.) 6, talc 5, and Mg stearate 5 mg.

د المجاري ريحُه (المعارية)

TT 120466-43-5 120466-44-6 122032-35-3 122032-36-4 167553-37-9 167553-38-0 167553-39-1 167553-40-4 167553-41-5

167553-42-6

RL: RCT (Reactant)

(antiarrhythmic phenylsulfonyldiazabicyclononanes)

RN 120466-43-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-ethyl-9,9-dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Me} & & & \\ & & & \\ & & \text{Me} & \\ \end{array}$$

RN 120466-44-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl-3-pentyl- (9CI) (CA INDEX NAME)

Me
$$\stackrel{\text{H N}}{\longrightarrow}$$
 $\stackrel{\text{N}}{\longrightarrow}$ (CH₂) 4 - Me

RN 122032-35-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9,9-dipropyl- (9CI) (CA INDEX NAME)

$$n-Pr$$
 N
 $Bu-n$
 $Pr-n$

RN 122032-36-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(cyclohexylmethyl)-9,9-dimethyl- (9CI) (CA INDEX NAME)

RN 167553-37-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9-methyl-9-propyl- (9CI) (CA INDEX NAME)

Page 124

RN 167553-38-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-hexyl-9-methyl-9-propyl- (9CI) (CA INDEX NAME)

$$n-Pr$$

N

(CH₂) 5-Me

RN 167553-39-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1] nonane, 9,9-dimethyl-3-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 167553-40-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,9-dibutyl-9-propyl- (9CI) (CA INDEX NAME)

$$n-Bu$$
 N
 $Bu-n$

RN 167553-41-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,9,9-tributyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 167553-42-6 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonane, 3-hexyl-9,9-dimethyl- (9CI) (CA INDEX NAME)

ANSWER 34 OF 97 CAPLUS COPYRIGHT 2001 ACS

N 1995:628110 CAPLUS

DN 123:228145

TI Structural, conformational, theoretical and pharmacological study of some amides derived from 3,7-dimethyl-9-(N-substituted 4-chlorobenzamido)-3,7-diazabicyclo[3.3.1]nonane-9-carboxamide

AU Fernandez, M. J.; Toledano, M. S.; Galvez, E.; Orjales, A.; Berisa, A.; Labeaga, L.; Fonseca, I.; Sanz-Aparicio, J.; Bellanato, J.

CS Departamento de Quimica Organica, Universidad de Alcala, 28871 Alcala de Henares, Madrid, Spain

SO J. Mol. Struct. (1995), 351, 137-46 CODEN: JMOSB4; ISSN: 0022-2860

DT Journal

LA English

GΙ

$$H_2NOC \longrightarrow N (CH_2R) CO \longrightarrow C1$$

MeN NMe

AB The title compds. (I; R = benzyl, Ph, 4-fluorophenyl) were prepd. and studied by IR, Raman, and 1H and 13C NMR spectroscopy and by mol. modeling techniques. The crystal structure of I (R = Ph) was detd. by x-ray diffraction. In CDCl3 and CD3OD solns., I adopt a nondistorted chair-chair conformation with the N-substituents in an equatorial position. I (R = Ph) prevented acetic acid-induced writhing in mice.

Ι

IT 168279-06-9

RL: PRP (Properties)
 (mol. modeling of)

RN / 168279-06-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-9-carboxamide, 9-[(4-chlorobenzoyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

ANSWER 35 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1995:441037 CAPLUS

DN 123:111879

TI Synthesis and biological activity of the metabolites of syn-3-ethyl-7-methyl-3,7-diazabicyclo[3.3.1]non-9-yl 4-chlorobenzoate hydrochloride

AU Yamawaki, Ichiro; Bukovac, Scott W.; Sunami, Akihiko

CS Tokushima Res. Cent., Pharmacokinetics Res. Lab. and Pharmacol. Res. Lab., Tokushima, 771-01, Japan

SO Chem. Pharm. Bull. (1994), 42(11), 2365-9 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

OS CASREACT 123:111879

AB Five metabolites of syn-3-ethyl-7-methyl-3,7-diazabicyclo[3.3.1]non-9-yl 4-chlorobenzoate hydrochloride (YUTAC) were prepd. and examd. for Na+ current blocking activity in guinea pig ventricular myocytes. These metabolites showed lower inhibitory activities than the parent compd. or were inactive.

IT 166272-89-5P 166272-90-8P 166272-91-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (synthesis and Na+ current blocking activity of the metabolites of Yutac)

RN 166272-89-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxylic acid, 9-[(4-chlorobenzoyl)oxy]-7-ethyl-, phenylmethyl ester, syn- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 166272-90-8 CAPLUS

CN Benzoic acid, 4-chloro-, 3-ethyl-3,7-diazabicyclo[3.3.1]non-9-yl ester, syn- (9CI) (CA INDEX NAME)

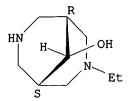
Relative stereochemistry.

RN 166272-91-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 3-ethyl-, syn- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Page 129



09/623,726 ANSWER 36 OF 97 CAPLUS COPYRIGHT 2001 ACS 1995:376577 CAPLUS 123:256562 DN-Synthesis and transformations of polyhedral compounds. 20. Synthesis of ΤI some derivatives of 3,7-diazabicyclo[3.3.1] nonane Minasyan, H. G.; Arutyunyan, A. D.; Adamyan, H. G.; Aghadrzhanyan, Ts. E. AU CS Inst. Tonkoi Org. Khim. im. A.L. Mndzhoyana, Yerevan, Armenia SO Khim. Geterotsikl. Soedin. (1994), (3), 401-6 CODEN: KGSSAQ; ISSN: 0132-6244 DTJournal Russian LА 1,3-Diazaadamantanes with CH2, CHOH, or C:NOH as position 6 reacted with AB aralkyl halides in aq. alk. media to give 3,7-diaralkyl-3,7diazabicyclo[3.3.1] nonanes with the above groups as position 9. A similar reaction of quaternary salts of 1,3-diazaadamantanes was also described. ΙT 169177-33-7P 169177-34-8P 169177-36-0P 169177-37-1P 169177-38-2P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 169177-33-7 CAPLUS RNなこのの 3,7-Diazabicyclo[3.3.1]nonane, 3-[(2-bromophenyl)methyl]-1,5-dimethyl-CN (CA INDEX NAME) Br HN CH₂ Me RN 169177-34-8 CAPLUS 3,7-Diazabicyclo[3.3.1]nonane, 3-[(3-bromophenyl)methyl]-1,5-dimethyl-CN (9CI) (CA INDEX NAME) Me HN Me RN 169177-36-0 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonane, 1,5-dimethyl-3-(phenylmethyl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME) CM 1 CRN 169177-19-9 CMF C16 H24 N2

CM 2

CRN 110-17-8 CMF C4 H4 O4 CDES 2:E

Double bond geometry as shown.

RN 169177-37-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-[(2-bromophenyl)methyl]-1,5-dimethyl-,
(2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 169177-33-7 CMF C16 H23 Br N2

CM 2

CRN 110-17-8 CMF C4 H4 O4 CDES 2:E

Double bond geometry as shown.

RN 169177-38-2 CAPLUS

Page 132

CM 2

CRN 110-17-8 CMF C4 H4 O4 CDES 2:E

Double bond geometry as shown.

IT 107606-88-2

RL: RCT (Reactant)
(prepn. of diazabicyclononanes from diazaadamantanes)

RN 107606-88-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

IT 169177-19-9P 169177-22-4P 169177-26-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of diazabicyclononanes from diazaadamantanes)

RN 169177-19-9 CAPLUS

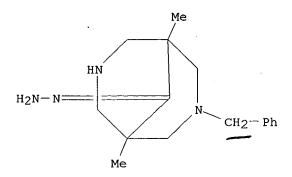
CN 3,7-Diazabicyclo[3.3.1]nonane, 1,5-dimethyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 169177-22-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-[(4-bromophenyl)methyl]-1,5-dimethyl-(9CI) (CA INDEX NAME)

RN 169177-26-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3-(phenylmethyl)-, hydrazone (9CI) (CA INDEX NAME)



ANSWER 37 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1995:376575 CAPLUS

DN 122:265351

TI Synthesis and transformations of polyhedral compounds. 18. Transformation of 1,3-diaza- and 1,3,5-triazaadamantanes into new nitrogen-containing polyhedral compounds by the action of dicarboxylic acid dichlorides

AU Aghadzhanyan, Ts. E.; Arutyunyan, G. L.; Adamyan, H. G.

CS Inst. Tonkoi Org. Khim. im. I.L. Mndzhoyana, Yerevan, Armenia

SO Khim. Geterotsikl. Soedin. (1994), (3), 393-6

CODEN: KGSSAQ; ISSN: 0132-6244

DT Journal

LA Russian

GΙ

AB Polyhedral compds. such as I, II, III, and IV were prepd. by reaction of di- and triazaadamantanes with phthaloyl and adipoyl chloride.

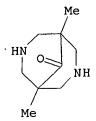
IT 80808-96-4

RL: RCT (Reactant)

(nitrogen-contg. polyhedral compds. from diaza- and triazaadamantanes and dicarboxylic acid dichlorides)

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)



3 ANSWER 38 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1994:700875 CAPLUS

DN 121:300875

TI Synthesis and transformations of polyhedric compounds. 17. Transformation of 1,3-diaza- and 1,3,5-triazaadamantanes to nitrogen-containing pentacyclic compounds

AU Minasyan, G. G.; Agadzhanyan, C. E.; Adamyan, G. G.

CS Inst. Tonk. Org. Khim., Yerevan, 375014, Armenia

SO Khim. Geterotsikl. Soedin. (1994), (1), 106-10

CODEN: KGSSAQ; ISSN: 0132-6244

DT Journal

LA Russian

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Reaction of diazaadamantane I (R = R1 = H, Me; R = H, R1 = Et) with diazabicyclononane II at high diln. in presence of Et3N afforded tetraaza pentacyclic compd. III (46-53%). Reaction of I with triazabicyclononane IV afforded pentaaza pentacyclic compd. V (52%), and of triazaadamantane VI with IV afforded hexaaza pentacyclic compd. VII (59%).

IT 80808-87-3

RL: RCT (Reactant)

(cycloalkylation reactions of 1,3-diaza- and 1,3,5-triazaadamantanes in prepn. of nitrogen-contg. pentacyclic compds.)

RN 80808-87-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(bromoacetyl)-1,5-dimethyl-(9CI) (CA INDEX NAME)

IT 80808-96-4P 147698-79-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (cycloalkylation reactions of 1,3-diaza- and 1,3,5-triazaadamantanes in prepn. of nitrogen-contg. pentacyclic compds.)

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)

RN 147698-79-1 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-diacetyl-1,5-dimethyl- (9CI) (CA INDEX NAME)

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09/623,726
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ANSWER 39 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1993:254788 CAPLUS

DN 118:254788

TI Synthesis and transformations of polyhedral compounds. 14. Opening of the hexahydropyrimidine ring of 2-substituted 1,3-diazaadamantanes by electrophilic reagents

AU. Agadzanyan, Ts.; Arutynyan, A. D.; Arutynyan, G. L.

CS Inst. Tonkor Org. Khim., Yerevan, 375014, Armenia

SO Khim. Geterotsikl. Soedin. (1992), (7), 929-32

CODEN: KGSSAQ; ISSN: 0132-6244

DT Journal

LA Russian

OS CASREACT 118:254788

GΙ

Reaction of diazaadamantanes I [R = H, R1 = Et, Ph, 3-pyridyl; R = R1 = H, Me; RR1 = (CH2)4] with Ac2O gave 80-92% diacetylated diazabicyclononane II (R2 = Ac). Treating I [R = H, R1 = Et, Ph, 3-pyridyl; R = R1 = Me; RR1 = (CH2)5] with aq. HONO gave 71-91% II (R2 = NO). Reaction of I (R = H, R1 = Et; R = R1 = Me) with BzCl or PhCH2Cl gave II (R2 = Bz, CH2Ph), resp.

IT 147698-79-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 147698-79-1 CAPLUS

CN *3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-diacetyl-1,5-dimethyl- (9CI) (CA INDEX NAME)

ANSWER 40 OF 97 CAPLUS COPYRIGHT 2001 ACS

1993:136694 CAPLUS

DN 118:136694

TI Crystal and molecular structure of 1,5-dimethyl-9,9-dihydroxy-3,7-diazabicyclo[3.3.1]nonane dihydrochloride dihydrate

AU Goncharov, A. V.; Potekhin, K. A.; Struchkov, Yu. T.; Svetlanova, A. M.; Chemodanova, S. V.; Palyulin, V. A.; Zefirov, N. S.

CS Mosk. Gos. Univ., Moscow, Russia

SO Dokl. Akad. Nauk (1992), 323(2), 285-9 [Chem.] CODEN: DAKNEQ

DT Journal

LA Russian

AB The title compd. is triclinic, space group P.hivin.1, with a 8.714(2), b 8.798(2), c 10.097(2) .ANG., .alpha. 77.67(2), .beta. 77.63(2), and .gamma. 82.39(2).degree.; dc = 1.44 for Z = 2. The at. coordinates are given. The structure was solved by direct methods and refined by least-squares to R = 0.059 and Rw = 0.0059. The bond lengths and angles are described. The H-bonding is depicted.

IT 146349-58-8, 1,5-Dimethyl-9,9-dihydroxy-3,7 diazabicyclo[3.3.1]nonane dihydrochloride dihydrate
 RL: PRP (Properties)
 (crystal structure of)

RN 146349-58-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-9,9-diol, 1,5-dimethyl-, dihydrochloride, dihydrate (9CI) (CA INDEX NAME)

•2 HCl

●2 H₂O

ANSWER 41 OF 97 CAPLUS COPYRIGHT 2001 ACS 1993:80837 CAPLUS 118:80837 DN Synthesis of 2,4,6,8-tetraphenyl-3,7-diazabicyclo[3.3.1]nonan-9-one from TI benzylideneacetone ΑU Kim, D. G.; Tulemisova, G. B.; Omarov, T. T. Inst. Khim. Nefti Prir. Solei, Gurev, Kazakhstan CS Zh. Org. Khim. (1992), 28(5), 1101-2 SO CODEN: ZORKAE; ISSN: 0514-7492 DTJournal Russian LΑ GΙ

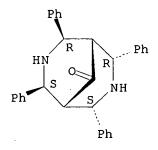
ANSWER 42 OF 97 CAPLUS COPYRIGHT 2001 ACS 1992:469818 CAPLUS DN 117:69818 ΤI A simple method for the preparation of 4,8,9,10-tetraphenyl-1,3diazaadamantanes Jeyaraman, R.; Ravindran, T.; Sujatha, M. ΑU Dep. Chem., Bharathidasan Univ., Tiruchirapalli, 620 024, India CS SO Indian J. Chem., Sect. B (1992), 31B(6), 362 CODEN: IJSBDB; ISSN: 0376-4699 DTJournal LA English OS CASREACT 117:69818

AΒ The title prepn. involves the reaction of aq. formaldehyde with 2,4,6,8-tetraaryl-3,7-diazabicyclo[3.3.1]nonanes. Yields of 78-83% were obtained.

ΙT 65732-77-6 75541-42-3 142698-37-1 RL: RCT (Reactant) (cyclocondensation of, with formaldehyde) RN 65732-7.7-6 CAPLUS

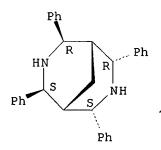
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl-, (2R, 4S, 6S, 8R) - rel - (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN75541-42-3 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetraphenyl-, (2-endo,4-endo,6exo, 8-exo) - (9CI) (CA INDEX NAME)

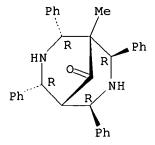
Relative stereochemistry.



RN 142698-37-1 CAPLUS 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl-, CN (2R, 4R, 6R, 8R) - rel - (9CI) (CA INDEX NAME)

ter on the partie

Relative stereochemistry.



ANA DN TI IN

ANSWER 43 OF 97 CAPLUS COPYRIGHT 2001 ACS

1992:440439 CAPLUS

DN 117:40439

TI Preparation of 3,7-diazabicyclo [3,3,1]nonanes as diuretics

IN Burow, Kurt; Buschmann, Gerd; Farjam, Arman; Kuehl, Ulrich; Varchmin, Gerda; Ziegler, Dièter; Schoen, Uwe

PA Kali-Chemie Pharma G.m.b.H., Germany

SO Eur. Pat. Appl., 16 pp.

CODEN: EPXXDW

DT Patent

LA German

FAN.CNT 1

FAN.CNT 1										
	PA:	TENT NO.		KIND	DATE		API	PLICATION N	O. DATE	
PΙ	ΕP	461574		A2	19911218		EP	1991-10944	9 19910608	
	EΡ	461574		A3	19920325					
	EP	461574		B1	19970924					
		R: AT, B	Ε, (CH, DE,	DK, ES,	FR,	GB,	GR, IT, LI,	LU, NL, SE	
	DE	4019080		A1	19911219		DE	1990-40190	80 19900615	
	ΑT	158583		E	19971015		AT	1991-10944	9 19910608	
	ES	2109244		Т3	19980116		ES	1991-10944	9 19910608	
	HU	58097		A2	19920128		HU	1991-1922	19910610	
	HU	210686		В	19950628					
	CA	2044673		AA	19911216		CA	1991-20446	73 19910614	
	ΑU	9178377		A1	19911219		AU	1991-78377	19910614	
	ΑU	640236		B2	19930819					
	JΡ	04230285		A2	19920819		JP	1991-14287	5 19910614	
	JΡ	3086007		B2	20000911					
	US	5164401		Α	19921117		US	1991-71488	6 19910617	
PRAI	DE	1990-40190	80	Α	19900615					
os	MAI	RPAT 117:40	439							
·GI										

$$R^{1}-N$$
 R^{2} R^{3} $N-R^{4}$ I

The 3,7-diazabicyclo[3.3.1]nonanes I [R1 = alkyl, alkenyl, cycloalkyl, benzyl; R2,R3 = alkyl; R2R3 = alkylene; R4 = (un)substituted phenylalkyl or diphenylmethane] are prepd. as diuretics. 3-Butyl-7-(2,5-dimethylbenzyl)-9,9-dimethyl-3,7-diazabicyclo[3.3.1]nonane (II) was prepd. by the reaction of 3-butyl-9,9-dimethyl-3,7-diazabicyclo[3.3.1]nonane with Li amide in DMF, followed by treatment with 2,5-dimethylbenzyl chloride in DMF. Oral administration of 10 mg II monosalicylate/kg had a strong diuretic effect in rats. Formulation examples are given.

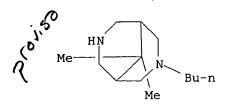
IT 120466-42-4

RL: BIOL (Biological study)

(condensation of, with dimethylbenzyl chloride)

RN 120466-42-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9,9-dimethyl- (9CI) (CA INDEX NAME)





LIV ANSWER 44 OF 97 CAPLUS COPYRIGHT 2001 ACS AN 1991:514550 CAPLUS

DN 115:114550

TI Preparation of salts of 3-azabicyclo[3.3.1]nonanes as antiarrhythmic agents

IN Berlin, Kenneth Darrell; Scherlag, Benjamin Jacob; Clarke, Cyril Roy; Otiv, Surendra Kamchandra; Zisman, Stan Alan; Sangiah, Subbiah; Mulekar, Satish Vasant

PA Oklahoma State University, USA

SO PCT Int. Appl., 68 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN. CNT 1

PAN.	FAN. CNT I															
	PAT	ENT I	NO.		KI	1D	DATE			AF	PLI	CATIO	ои ис	э.	DATE	
PI	WO	9107	405 JP		A.	 L	1991	0530		WC	19	90-U	s662	5	1990	1113
				BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LU,	NL,	SE	
	US	5084	572		A		1992	0128		JU.S	198	89-43	3597	6	1989	1113
	US	51109	933		Α		1992	0505		US	199	90-63	1042	8	1990	1107
PRAI	US	1989-	-4359	976			1989	1113								
	US	1990-	-6104	128			1990	1107								
os	MAI	RPAT :	115:1	1455	0											
GI					•											

AB * Title compds. [I; HX = pharmacol. acceptable acid; Q = CH2, CO; Y = S, SO, CHCO2Et, NR1; Z = CH2, CO, C(OMe)2, Q1; R = H, alkyl, (substituted) PhCH2, PhCO; PhSO2, Q1; R1 = alkyl, (substituted) PhCH2, PhCO], were prepd. 7-Benzyl-3-isopropyl-3,7-diazabicyclo[3.3.1]nonane (prepn. from 1-isopropyl-4-piperidinone given) was refluxed with Pd/HCO2NH4 in MeOH to give the unprotected amine; the latter was acylated with PhCOCl in 10% NaOH/CH2Cl2 and the product was converted to perchlorate salt II. Several I at 3 mg/kg in dogs effectively eliminated induced ventricular tachycardia.

IT 129039-76-5P

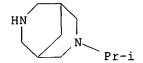
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

1 4 . Land Bridge 12 . Land

(prepn. of, as antiarrhythmic)

RN 129039-76-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-methylethyl)- (9CI) (CA INDEX NAME)



A3 ANSWER 45 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1991:449662 CAPLUS

DN 115:49662

TI Synthesis and transformation of polyhedric compounds. XIII. Search for antitumor agents among indolyl-1,3-diazaadamantanes

AU Chachoyan, A. A.; Shkulev, V. A.; Pisarskii, Yu. B.; Saakyan, G. S.;

Agadzhanyan, Ts. E.; Garibdzhanyan, B. T.

CS Inst. Tonkoi Org. Khim., Yerevan, USSR

SO Khim.-Farm. Zh. (1991), 25(4), 45-8

CODEN: KHFZAN; ISSN: 0023-1134

DT Journal

LA Russian

GΙ

HN

HN

AB The title compds. I (R, R1 = H, Me; R2 = H, OMe, dialkylaminosulfonyl) were prepd. by cyclocondensation of formylindoles II with diazabicyclononanone III in 52-67% yield. Their antitumor activity was examd.

III

ΙI

IT 80808-96-4

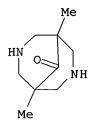
RL: RCT (Reactant)

(cyclocondensation of, with formylindoles)

Me

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)



ANSWER 46 OF 97 CAPLUS COPYRIGHT 2001 ACS AN 1991:122245 CAPLUS DN 114:122245

TI An improved synthesis of 4,8,9,10-tetraaryl-1,3-diazaadamantanes

AU Sivasubramanian, S.; Sundaravadivelu, M.; Arumugam, N.

CS Dep. Org. Chem., Madurai Kamaraj Univ., Madurai, 625 021, India

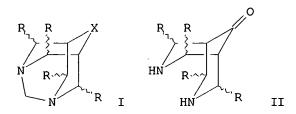
SO Org. Prep. Proced. Int. (1990), 22(5), 645-8

CODEN: OPPIAK; ISSN: 0030-4948

DT Journal LA English

OS CASREACT 114:122245

GΙ



AB The diazaadamantanes I (R = Ph, 4-MeC6H4, X = CH2) were prepd. by Wolff-Kishner redn. of the corresponding I (X = CO) which were prepd. by cyclocondensation diazabicyclononanones II with paraformaldehyde in DMSO.

IT 37123-09-4 55407-47-1 60823-94-1 77737-97-4 77841-40-8

RL: RCT (Reactant)

(cyclocondensation of, with paraformaldehyde, diazaadamantanone from)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 55407-47-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methoxyphenyl)-(9CI) (CA INDEX NAME)

RN 60823-94-1 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 77737-97-4 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-chlorophenyl)(9CI) (CA INDEX NAME)

RN 77841-40-8 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methylphenyl)-(9CI) (CA INDEX NAME)

MSWA

ANSWER 47 OF 97 CAPLUS COPYRIGHT 2001 ACS

1991:121397 CAPLUS

5N \114:121397

TI Synthesis and reactions of polyhedric compounds. XI. Synthesis and antitumor activity of new derivatives of 3,7-diaza- and 1,3,7-triazabicyclo[3.3.1]nonanes

AU Minasyan, G. G.; Saakyan, G. S.; Agadzhanyan, Ts. E.; Chachoyan, A. A.; Garibdzhanyan, B. T.

CS Inst. Tonk. Org. Khim., Yerevan, USSR

SO Arm. Khim. Zh. (1990), 43(2), 107-12 CODEN: AYKZAN; ISSN: 0515-9628

DT Journal

LA Russian

GΙ

Me NO2
NR NR NR1

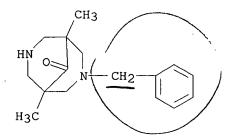
AB Treating diazabicyclononanone I (R = R1 = H) with epichlorohydrin, 3-phenoxy-1,2-epoxypropane, PhNCS, or ClCH2CN gave disubstituted I [R = CH2CH(OH)CH2Cl, CH2CH(OH)CH2OPh, CSNHPh, CH2CN] and monosubstituted I (R = CSNHCH2CH:CH2, COCH:CHCO2H, COCH2CH2CO2H) when treated with allyl isothiocyanate, maleic or succinic anhydrides. Addnl. obtained were triazabicyclononanes II (R2 = HC.tplbond.CCH2, COMe, CSNHPh, R3 = PhCH2; R2 = CSNHPh R3 = HC.tplbond.CCH2). I and II were useful neoplasm inhibitors against sarcoma 45 and Ehrlich's carcinoma.

IT 107606-88-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and addn. reaction with Ph isothiocyanate)

RN - 107606-88-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 132401-96-8P

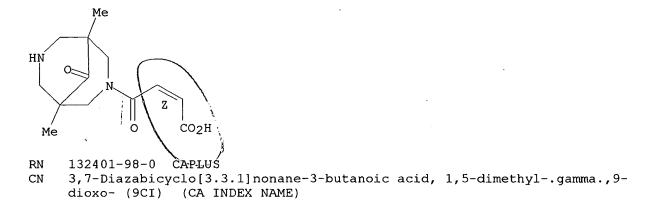
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and toxicity of)

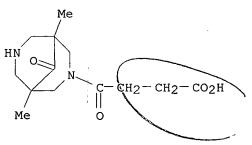
RN 132401-96-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, 1,5-dimethyl-9-oxo-N-2-

propenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





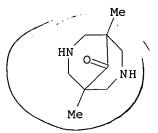
IT 80808-96-4

RL: RCT (Reactant)

(substitution and addn. reactions of)

RN 80808-96-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)



3 ANSWER 48 OF 97 CAPLUS COPYRIGHT 2001 ACS

1990:532149 CAPLUS

DN 113:132149

TI A study of the synthesis and antiarrhythmic properties of selected 3,7-diheterabicyclo[3.3.1]nonanes with substituents at the 2,4-positions and at the 9-position

AU Smith, Gary Steven; Thompson, Mark Daniel; Berlin, Kenneth Darrell; Holt, Elizabeth Manners; Scherlag, Benjamin Jacob; Patterson, Eugene; Lazzara, Ralph

CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA

SO Eur. J. Med. Chem. (1990), 25(1), 1-8 CODEN: EJMCA5; ISSN: 0223-5234

DT Journal

LA English

OS CASREACT 113:132149

GΙ

AB Some members of the family of 3,7-diheterabicyclo[3.3.1]nonanes I (X = S, R = OMe, R1 = H; X = NCH2Ph, R = OH, OMe, R1 = H; X = NH, R = H, R1 = 2-ClC6H4) and II with substituents at the 2-, 4- and 9-positions were synthesized via Mannich reaction. Hearts of anesthetized dogs with myocardial infarctions were subjected to ventricular tachycardia (VT). I and II exhibited ability to abolish VT [or prevent the VT from being sustained] or reduce the rate of VT. A CH2 group at the 9-position or the Me ketal group [(MeO)2C(9)] enhanced the antiarrhythmic activity regardless of whether S or N was at 3-position. Compds. with aryl groups alpha to the heteroatoms were less effective in controlling VT. Lidocaine was the std.

IT 118958-21-7P

RN 118958-21-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, (endo,endo)- (9CI) (CA INDEX NAME)

IT 118958-24-0P

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn., crystal structure, nitrogen NMR, and antiarrhythmic activity of)

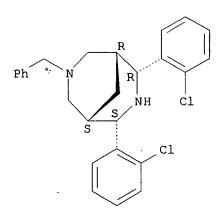
RN 118958-24-0 CAPLUS

3,7-Diazabicyclo[3.3.1]nonane, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, (endo,endo)-, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 118958-23-9 CMF C26 H26 C12 N2 CDES 2:ENDO,ENDO

Relative stereochemistry.



CM 2

CRN 7601-90-3 CMF Cl H O4

IT 118958-23-9P

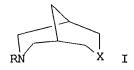
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn., nitrogen NMR, and reaction of, with perchloric acid, conformation and antiarrhythmic activity of)

RN 118958-23-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, (endo,endo)- (9CI) (CA INDEX NAME)

ANSWER 49 OF 97 CAPLUS COPYRIGHT 2001 ACS 1990:515277 CAPLUS /DN 113:115277 The preparation of amide derivatives of 3-azabicyclo[3.3.1] nonanes as new TI potential antiarrhythmic agents ΑU Zisman, Stan A.; Berlin, K. Darrell; Scherlag, B. J. Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74074, USA CS Org. Prep. Proced. Int. (1990), 22(2), 255-64 SO CODEN: OPPIAK; ISSN: 0030-4948 DTJournal LΑ English OS CASREACT 113:115277

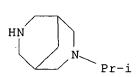


GΙ

AB The title compds. I [X = S, R = Bz; X = NCHMe2, R = Bz, 4-ClC6H4CO, 3,4-(MeO)2C6H3CO, 3,4,5-(MeO)3C6H2CO, PhSO2] were prep. from 4-thianone and 1-isopropyl-4-piperidinone.

IT 129039-76-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and acylation or sulfonation of)
RN 129039-76-5 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-methylethyl)- (9CI) (CA INDEX NAME)





ANSWER 50 OF 97 CAPLUS COPYRIGHT 2001 ACS 1990:515129 CAPLUS 113:115129 ΤI Part I. Synthesis and antiarrhythmic properties of substituted 3,7-diazabicyclo[3.3.1]nonanes and 3-azabicyclo[3.3.1]nonanes, and derivatives. Part II. Oxygen-17 NMR analysis of substituted 1-hetera-4-cyclohexanones ΑU Mulekar, Satish Vasant CS Oklahoma State Univ., Stillwater, OK, USA SO (1989) 181 pp. Avail.: Univ. Microfilms Int., Order No. DA9004033 From: Diss. Abstr. Int. B 1990, 50(9), 3997 DTDissertation LΑ English AΒ Unavailable ΙT 280-74-ODP, 3,7-Diazabicyclo[3.3.1] nonane, derivs. RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and antiarrhythmic activity of) 280-74-0 CAPLUS RN

3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)



CN

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09/62/3,726
     ANSWER 51 OF 97 CAPLUS COPYRIGHT 2001 ACS
     1990:20978 CAPLUS
DN
     112:20978
ΤI
     Synthesis, stereochemistry and analgesic activity of 3,7-
     diazabicyclo[3.3.1]nonan-9-ones and 1,3-diazaadamantan-6-ones
     Samhammer, Annemarie; Holzgrabe, Ulrike; Haller, Rolf
ΑU
     Pharm. Inst., Univ. Kiel, Kiel, 2300, Fed. Rep. Ger.
CS
     Arch. Pharm. (Weinheim, Ger.) (1989), 322(9), 551-5
SO
     CODEN: ARPMAS; ISSN: 0365-6233
DT
     Journal
     German
LА
OS
     CASREACT 112:20978
GI
```

The 1,3-diazaadamantan-6-ones I (R = 2-pyridyl, 6-methyl-2-pyridyl, Ph, AΒ 3,4,5-Me3C6H2, R1R2 = CH2) are synthesized from the 4-piperidones II. Different conditions lead to stereoisomeric structures. The 3,7-diazabicyclo[3.3.1]nonan-9-ones I (R1 = H, Me, R2 = Me, cyclopropylmethyl, R = same) show similar geometrical isomerism. Whereas the diazabicyclononanes show opioid-like effects, I (R = 2-pyridyl, R1R2 = CH2) is a peripheral analgesic. IT 124189-56-6P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) RN 124189-56-6 CAPLUS 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-(cyclopropylmethyl)-CN 9-oxo-2,4-di-2-pyridinyl-, dimethyl ester, (endo,endo)- (9CI) (CA INDEX

Relative stereochemistry.

NAME)

09/623,726

ANSWER 52 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1990:20977 CAPLUS

DN 112:20977

TI Reductions of 3,7-diazabicyclo[3.3.1]nonan-9-ones and corresponding 1,3-diazaadamantan-6-ones

AU Samhammer, Annemarie; Holzgrabe, Ulrike; Haller, Rolf

CS Pharm. Inst., Univ. Kiel, Kiel, 2300, Fed. Rep. Ger.

SO Arch. Pharm. (Weinheim, Ger.) (1989), 322(9), 545-50

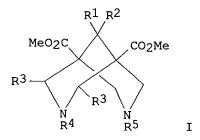
CODEN: ARPMAS; ISSN: 0365-6233

DT Journal

LA German

OS CASREACT 112:20977

GI



AB The title compds. I (R1R2 = O, R3 = 2-pyridyl, Ph, 6-methyl-2-pyridyl, R4 = H, Me, R5 = Me, Et; R4R5 = CH2, resp.) are reduced by NaBH4 and LiAlH4 in various solvents. The reasons for the proportion of the epimeric alcs. are discussed. The reaction of I (R1R2 = O, R3 = Ph, R4R5 = CH2) with MeMgI yields the ring-opened N-alkylated product.

IT 124189-67-9P

RN 124189-67-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-ethyl-9-oxo-2,4-diphenyl-, dimethyl ester, (endo,endo)- (9CI) (CA INDEX NAME)

ANSWER 53 OF 97 CAPLUS COPYRIGHT 2001 ACS

1989:515218 CAPLUS

DN 111:115218

ΤI Preparation and testing of bispidin derivatives as class III antiarrhythmics

IN Lubisch, Wilfried; Binnig, Fritz; Von Philipsborn, Gerda

BASF A.-G., Fed. Rep. Ger.

SO Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

DT Patent

LΑ German

PA

FAN.	CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	EP 308843	A2	19890329	EP 1988-115299	19880917
	EP 308843	А3 -	19900808		
	EP 308843	B1	19931215		
	R: BE, CH,	DE, FR	, GB, IT, LI,	NL, SE	
	DE 3732094	A1	19890406	DE 1987-3732094	19870924
	JP 01102078	A2 -	19890419	JP 1988-235124	19880921
	US 4959373	Α	19900925	US 1988-247645	19880922
PRAI	DE 1987-3732094		19870924		
os	MARPAT 111:1152	18			
GT					

ΑB The title compds. (I; R, R1, R3 = H, C1-4 alkyl, halo, C1-4 alkoxy; R2 = C1-4 alkyl halo, CN, C1-4 alkoxy NHS, 2Me, CF3 NHCOMe, amino, NO2; X = CH2, CO, CR4OR5; R4 = H, C1-4 alkyl; R5 = R4, Q1; R6 = R4, halo, C1-4 alkoxy; Y = CO, CONH; Z = C1-4 alkylene), were prepd. 3-(4-Aminobenzoyl)-7-benzyl-3,7-diazabicyclo[3.3.1] nonane in THF at ice temp. was treated with AcCl in THF and then with Et3N at room temp. The mixt. was stirred overnight to give 3-(4-acetaminobenzoyl)-7-benzyl-3,7-diazabicyclo[3.3.1]nonane. I in guinea pigs showed prolongation of QT times with ED20's of 2.4-4.6 mg/kg i.v.

IT 69407-32-5

RL: RCT (Reactant)

(acylation of, in prepn. of antiarrhythmics)

RN69407-32-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)

IT 122455-78-1

RL: RCT (Reactant)

09/623,726

(condensation of, with chlorobenzyl bromide, in prepn. of antiarrhythmics)

RN 122455-78-1 CAPLUS

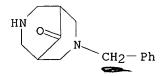
CN Acetamide, N-[4-(3,7-diazabicyclo[3.3.1]non-3-ylcarbonyl)phenyl]- (9CI) (CA INDEX NAME)

IT 122455-82-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and condensation of, with chlorobenzoyl chloride, in prepn. of antiarrhythmics)

RN 122455-82-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT : 122455-80-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and hydrogenation of, in prepn. of antiarrhythmics)

RN 122455-80-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(4-nitrophenyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

IT 122455-61-2P 122455-62-3P 122455-63-4P

122455-64-5P 122455-65-6P 122455-66-7P

122455-67-8P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as antiarrhythmic)

RN 122455-61-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(4-methylphenyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

09/623,726

RN 122455-62-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(4-methoxyphenyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 122455-63-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(4-chlorophenyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 122455-64-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-phenyl-7-(phenylmethyl)-(9CI) (CA INDEX NAME)

RN 122455-65-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(4-aminophenyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 122455-66-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[(4-chlorophenyl)methyl]-N-phenyl- (9CI) (CA INDEX NAME)

RN 122455-67-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 7-[(4-nitrophenyl)methyl]-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

• HCl

IT 122455-81-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as intermediate for antiarrhythmics)

RN 122455-81-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-phenyl- (9CI) (CA INDEX NAME)

Page 167

ΙT 122455-64-5

RL: RCT (Reactant) (reaction of, in prepn. of antiarrhythmics) 122455-64-5 CAPLUS

RN

3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-phenyl-7-(phenylmethyl)-CN(9CI) (CA INDEX NAME)

C-NHPh

ANSWER 54 OF 97 CAPLUS COPYRIGHT 2001 ACS AN 1989:478039 CAPLUS

DN 111:78039

TI Preparation and testing of 3-cinnamyl or 3-benzhydryl-3,7-diazabicyclo[3.3.1]nonanes as bradycardiacs and antiarrhythmics

IN Schoen, Uwe; Kehrbach, Wolfgang; Buschmann, Gerd; Kuehl, Ulrich Gottfried; Ziegler, Dieter

PA Kali-Chemie Pharma G.m.b.H., Fed. Rep. Ger.

SO Eur. Pat. Appl., 31 pp.

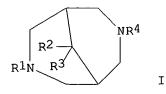
CODEN: EPXXDW

DT Patent

LA German

FAN.CNT 1

r Pan . v		TENT NO.	KIND	DATE		APPLICATION NO. DATE	
ΡI	EP	306871		19890315		EP 1988-114428 19880903	,
	EΡ	306871	A3	19900801		•	
	ΕP	306871	B1	19931208			
		R: AT, BE,	CH, DE	, ES, FR, (GΒ,	GR, IT, LI, LU, NL, SE	•
	DE	3730224	A1			DE 1987-3730224 19870909)
	DE	3730222	A1	19890330		DE 1987-3730222 19870909)
	US	4912113	Α	19900327		US 1988-239766 19880902	
	ES	2061580	Т3	19941216		ES 1988-114428 19880903	;
	ZA	8806619	Α	19890530		ZA 1988-6619 19880906	í
	JP	01068372	A2	19890314		JP 1988-222583 19880907	1
	HU	48248	A2	19890529		HU 1988-4606 19880907	1
	HU	198718	В	19891128			
	DD	282228	A 5	19900905		DD 1988-319603 19880907	1
	FI	8804138	Α	19890310		FI 1988-4138 19880908	,
	DK	8804989	Α	19890310		DK 1988-4989 19880908	į
	NO	8804008	Α	19890310		NO 1988-4008 19880908)
	ΑU	8822005	A1	19890323		AU 1988-22005 19880908	ł
	ΑU	605904	B2	19910124			
PRAI	DE	1987-3730222		19870909			
	DE	1987-3730224		19870909			
os	MAI	RPAT 111:7803	9				
GI							



The title compds. [I; R1 = C1-6 alkyl, C4-9 cycloalkyl, PhCH2; R2,R3 = lower alkyl; R2R3 = C3-6 alkylene; R4 = (substituted) Ph2CH, PhCH:CHCH2], useful as antiarrhythmics and bradycardiacs, were prepd.

3-Butyl-9,9-dimethyl-3,7-diazabicyclo[3.3.1]nonane, Ph2CHBr, and K2CO3 were stirred 12 h in DMF to give 7-diphenylmethyl-3-n-butyl-9,9-dimethyl-3,7-diazabicyclo[3.3.1]nonane. I at 10 .mu.mol/kg i.v. in rats decreased pulse by 27-49% while changing blood pressure by -11 to +11%.

IT 120466-46-8

RL: RCT (Reactant)

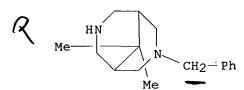
(acylation of, by cinnamoyl chloride, in prepn. of antiarrhythmic-

09/623,726

bradycardiac)

RN 120466-46-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



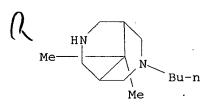
IT 120466-42-4 122032-37-5 122032-38-6

RL: RCT (Reactant)

(condensation of, with diphenylmethylbromide, in prepn. of antiarrhythmic-bradycardiac)

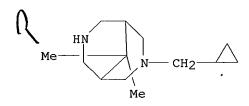
RN 120466-42-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9,9-dimethyl- (9CI) (CA INDEX NAME)



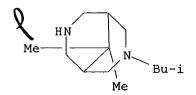
RN 122032-37-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(cyclopropylmethyl)-9,9-dimethyl- (9CI) (CA INDEX NAME)



RN 122032-38-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl-3-(2-methylpropyl)- (9CI) (CA INDEX NAME)



IT 120466-42-4P 120466-46-8P 122032-35-3P

Page 170

122032-36-4P 122032-37-5P 122032-38-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as intermediate for antiarrhythmic and bradycardiac)

RN 120466-42-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9,9-dimethyl- (9CI) (CA INDEX NAME)

$$Me$$
 HN
 N
 $Bu-n$
 Me

RN 120466-46-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 122032-35-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9,9-dipropyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ n-Pr & & & \\ & & & \\ N & & \\ N & & \\ Bu-n & \\ Pr-n & \\ \end{array}$$

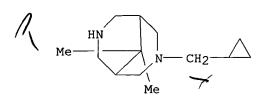
RN 122032-36-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(cyclohexylmethyl)-9,9-dimethyl- (9CI) (CA INDEX NAME)

RN 122032-37-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(cyclopropylmethyl)-9,9-dimethyl- (9CI) (CA INDEX NAME)

Page 171



RN 122032-38-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl-3-(2-methylpropyl)- (9CI) (CA INDEX NAME)

ANSWER 55 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1989:415252 CAPLUS

DN 111:15252

TI Improving the lightfastness of colored organic materials

IN Kaneko, Yutaka

PA Konica Co., Japan

SO Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI GI	JP 63281158	A2	19881117	JP 1987-116326	19870513

AB In the title method, an org. colored material and I [R1, R2 = H, alkyl, cycloalkyl, alkenyl, cycloalkenyl, alkynl, aryl, heterocycycl, acyl, sulfonyl, carbamoyl, phosphonyl, sulfamoyl, oxycarbonyl; R3 = substituent; m = 0-6] are allowed to coexist. The method is esp. useful in color photog., inks and fabric dyes. A photog material contained I [R1 = CH3; R2 = C6H5CH2] and a magenta dye to prevent photofading.

IT 69407-32-5 121171-74-2 121171-79-7

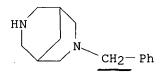
Ι

RL: USES (Uses)

(lightfastness improvement additive, for orgs.)

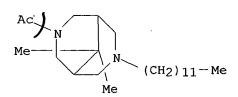
RN 69407-32-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 121171-74-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-acetyl-7-dodecyl-9,9-dimethyl- (9CI) (CA INDEX NAME)



Page 173

RN 121171-79-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-[[2,4-bis(1,1-dimethylpropyl)phenoxy]acetyl]-7-hexadecyl- (9CI) (CA INDEX NAME)

ANSWER 56 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1989:212804 CAPLUS

DN 110:212804

TI Preparation of 3-sulfonyl-3,7-diazabicyclo[3.3.1]nonanes as stomach motility stimulants

IN Schoen, Uwe; Kehrbach, Wolfgang; Wolf, Klaus Ullrich

PA Kali-Chemie Pharma G.m.b.H., Fed. Rep. Ger.

SO Ger. Offen., 13 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

CAIN.	CNII					
	PATENT NO.	KIND	DATE	AP:	PLICATION NO.	DATE
ΡI	DE 3722134	A1	19890119	DE	1987-3722134	1.9870704
	EP 301245	A2	19890201	EP	1988-110180	19880625
	EP 301245	A3	19890524		• .	
	EP 301245	B1	19930908			
	R: BE, CH,	DE, FR	, GB, IT, LI,	NL	•	
	JP 01029377	A2	19890131	JP	1988-159562	19880629
	US 4906640	Α	19900306	US	1988-214032	19880630
	US 4983611	Α	19910108	US	1989-401749	19890925
PRAI	DE 1987-3722134		19870704			
	US 1988-214032		19880630			
os	MARPAT 110:21280)4				
GI						

$$R^{1}N$$
 R^{2} R^{3} $NSO_{2}R^{4}$ R^{3} $NSO_{2}R^{4}$ R^{2} R^{3} $NSO_{2}R^{4}$ R^{3} R^{2} R^{3} $NSO_{2}R^{4}$ R^{3} R^{2} R^{3} R^{3} R^{2} R^{3} R

The title compds. [I; R1 = alkyl, cycloalkyl, PhCH2; R2, R3 = H, alkyl; R2R3 = C3-6 alkylene; R4 = alkyl, thienyl, halothienyl, (CH2)nR5; R5 = (un)substituted Ph; n = 0-3] were prepd. Tetraoxodiazabicyclononane II (R1 = Bu, R2 = R3 = Me) (prepn. described) was reduced and deprotected to give 7-butyl-9,9-dimethyl-3,7-diazabicyclo[3.3.1]nonane which was stirred 3 h with 3,4-Cl2C6H3SO2Cl in CH2Cl2 to give I.HCl (R1 = Bu, R2 = R3 = Me, R4 = 3,4-Cl2C6H3) (III) which increased the amplitude of rat gastric peristalsis >10-fold at 100 .mu.mol/kg i.p. Tablets were prepd. each contg. III 20, starch 69, lactose 135, gelatin 6, talc 5, and Mg stearate 5 mg.

IT 120466-42-4P 120466-43-5P 120466-44-6P 120466-46-8P 120482-82-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction of, in prepn. of stomach motility stimulants)

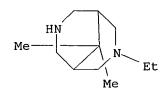
RN 120466-42-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-9,9-dimethyl- (9CI) (CA INDEX NAME)

$$\bigwedge_{\mathsf{Me}}^{\mathsf{HN}} \bigvee_{\mathsf{Ne}}^{\mathsf{N}} \bigvee_{\mathsf{Bu-n}}^{\mathsf{Bu-n}}$$

RN 120466-43-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-ethyl-9,9-dimethyl- (9CI) (CA INDEX NAME)



RN 120466-44-6 CAPLUS

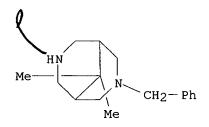
CN 3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl-3-pentyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c}
\begin{array}{c}
\text{Me} \\
\text{Me}
\end{array}$$

$$\begin{array}{c}
\text{N} \\
\text{CH2} \\
\text{Me}
\end{array}$$

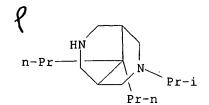
RN 120466-46-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 9,9-dimethyl-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 120482-82-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(1-methylethyl)-9,9-dipropyl- (9CI) (CA INDEX NAME)



3 ANSWER 57 OE 97 CAPLUS COPYRIGHT 2001 ACS

1989:95288 CAPLUS

DN 110:95288

TI Preparation of 3-selena-7-azabicyclo[3.3.1]nonanes as antiarrhythmic agents

IN Berlin, Kenneth D.; Thompson, Mark D.; Scherlag, Benjamin J.; Smith, Gary S.

PA Oklahoma State University, USA

SO U.S., 24 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

FAN.CNT 1									
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
		-							
ΡI	US 4778892	Α	19881018	US 1987-48325	19870511				
	US 4910311	Α	19900320	US 1988-222057	19880708				
	US 4980468	Α	19901225	US 1989-448658	19891211				
	US 5043445	Α	19910827	US 1990-596550	19901115				
	US 5268481	Α	19931207	US 1991-706215	19910528				
PRA	I US 1987-48325		19870511						
	US 1988-222057		19880708						
	US 1989-448658		19891211	•					
	US 1990-596550	•	19901115						
os	MARPAT 110:95288								
GI									

The title compds. [I; R = Ph, PhCH2, 4-MeOC6H4CH2, 3,4-(MeO)2C6H3CH2, 2-thienyl; X = CO, CH2, C(OH)2, C(OMe)2] and their aza, oxa, and thia analogs and salts were prepd. as antiarrhythmics. PhCH2NH2, paraformaldehyde, HOAc, and 4-selenanone were refluxed in MeOH to give 43% exo-I (R = Ph, X = CO) which was heated 12 h at 140.degree. with N2H4 in triethylene glycol to give, after acidification, 75% endo-I.HClO4 (R = Ph, X = CH2) (II). I reduce or eliminate artificially induced, sustained ventricular tachycardia in dogs at 3 and 6 mg/kg, their effect being superior to that of lidocaine.

IT 118958-20-6P 118958-21-7P 118958-22-8P 118958-23-9P 118958-24-0P 119001-04-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as antiarrhythmic)

RN 118958-20-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, (exo,exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Page 178

RN 118958-21-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, (endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 118958-22-8 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, . (exo,exo)- (9CI) (CA INDEX NAME)

RN 118958-23-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, (endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 118958-24-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, (endo,endo)-, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 118958-23-9 CMF C26 H26 C12 N2 CDES 2:ENDO,ENDO

CM 2

CRN 7601-90-3 CMF Cl H O4

RN 119001-04-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4-bis(2-chlorophenyl)-7-(phenylmethyl)-, (exo,exo)-, monoperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 118958-22-8 CMF C26 H26 C12 N2 CDES 2:EXO,EXO

Page 181

CM 2

CRN 7601-90-3 CMF Cl H O4

ANSWER 58 OF 97 CAPLUS COPYRIGHT 2001 ACS

1987:439733 CAPLUS

107:39733 DΝ

Synthesis and transformations of polyhedral compounds. X. Synthesis of ΤI 2-substituted 5,7-dimethyl-1,3-diazaadamantan-6-ones

Saakyan, G. S.; Arutyunyan, G. L.; Agadzhanyan, Ts. E.; Paronikyan, R. V. ΑU

CS

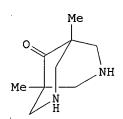
Inst. Tonk. Org. Khim., Yerevan, USSR Arm. Khim. Zh. (1986), 39(4), 242-6 SO CODEN: AYKZAN; ISSN: 0515-9628

Journal \mathbf{DT}

Russian LA

CASREACT 107:39733 OS

GΙ



Me II

Condensation of diazabicyclononanone I with aldehydes and ketones gave 26 AΒ title compds. II [e.g., R, R1, and % yield given: 2-FC6H4, H, 70; 5,2-Br(HO)C6H3, H, 42; 3-pyridyl, H, 62; Et, H, 91; RR1 = (CH2)4, 68].

IT 80808-96-4

RL: RCT (Reactant)

Ι

(cyclocondensation of, with aldehydes and ketones)

RN80808-96-4 . CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)

```
09//623,726
     ANSWER 59 OF 97 CAPLUS COPYRIGHT 2001 ACS
      1987:156393 CAPLUS
ΑN
      106:156393
DN
      Preparation and reactions of polyhedral compounds. IX. Reaction of
ΤI
      1,3-diaza- and 1,3,5-triazaadamantanes with halo compounds
     Minasyan, G. G.; Mkrtchyan, M. B.; Agadzhanyan, Ts. E. Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
ΑU
CS
SO
     Arm. Khim. Zh. (1986), 39(1), 44-8
     CODEN: AYKZAN; ISSN: 0515-9628
DT
      Journal
LΑ
     Russian
OS
     CASREACT 106:156393
```

GI

09/623,726 ANSWER 60 OF 97 CAPLUS COPYRIGHT 2001 ACS 1986:5249 CAPLUS 104:5249 DN Conformational studies of some bicyclo[3.3.1]nonan-9-ones using dipole ΤI moments and PMR spectra Pandiarajan, K.; Stalin, K. K. ΑU CS Dep. Chem., Annamalai Univ., Annamalainagar, 608 002, India Indian J. Chem., Sect. B (1985), 24B(5), 565-7 SO CODEN: IJSBDB; ISSN: 0376-4699 DΤ Journal English LА

Dipole moments of 2,4-diphenyl-3-azabicyclo[3.3.1]nonan-9-one (I), 2,4, 6,8-tetraphenyl-3-thia-7-azabicyclo[3.3.1]nonan-9-one [II; X = S(III)]and 2,4,6,8-tetraphenyl-3-azabicyclo[3.3.1]nonan-9-one [II; X = CH2(IV)] detd. in dioxane, indicate that the N-contg. ring is in the chair form in I, but in the boat form in III and IV; the N atom lone pair in these compds. is in the flagpole position. The 1H NMR of I indicates chair conformation for the cyclohexane ring. The 1H NMR of 2,4,6,8-tetraphenyl-3,7-diazabicyclo[3.3.1]nonan-9-one (II; X = NH) and III show chair-boat structure for these compds.

GI

√ 3 ANSWER 61 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1985:453976 CAPLUS

DN 103:53976

TI Reductions of substituted 3,7-diaza- and 3-thia-7-azabicyclo[3.3.1]nonan-9-ones with sodium borohydride

AU Haller, Rolf; Ashauer, Ulrike

CS Pharm. Inst., Univ. Kiel, Kiel, 2300/1, Fed. Rep. Ger.

SO Arch. Pharm. (Weinheim, Ger.) (1985), 318(5), 405-10 CODEN: ARPMAS; ISSN: 0365-6233

DT Journal

LA German

OS CASREACT 103:53976

GI For diagram(s), see printed CA Issue.

AB Redn. of bicyclononanones I (X = NH, R1 = Ph, 2-pyridyl, R2 = Me; X = NH, R1 = 2-pyridyl, R2 = CH2Ph; X = S, R1 = 2-pyridyl, R2 = Me) with NaBH4 in aq. dioxane was highly stereoselective, to give the axial bicyclononanols II (R3 = OH, R4 = H). In MeOH, NaBH4 redn. gave mixts. of epimers II (R3 = OH, R4 = H; R3 = H, R4 = OH).

IT 36332-85-1P 97323-52-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by redn. of oxo analog with sodium borohydride)

RN 36332-85-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-hydroxy-7-(phenylmethyl)-2,4-di-2-pyridinyl-, dimethyl ester, (endo,endo,syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 97323-52-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-hydroxy-7-(phenylmethyl)-2,4-di-2-pyridinyl-, dimethyl ester, (endo,endo,anti)-(9CI) (CA INDEX NAME)

IT 97323-46-1
 RL: RCT (Reactant)
 (redn. of, with sodium borohydride, stereochem. in relation to solvent)
RN 97323-46-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-7 (phenylmethyl)-2,4-di-2-pyridinyl-, dimethyl ester, (endo,endo)- (9CI)
 (CA INDEX NAME)

ANSWER 62 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN - 1984:570576 CAPLUS

DN 101:170576

TI 2,6-Diphenylpiperidine systems - a PMR spectral study

AU Sivasubramanian, S.; Sundharavadivelu, M.; Arumugam, N.

CS Dep. Org. Chem., Madurai Kamaraj Univ., Madurai, 625 021, India

Indian J. Chem., Sect. B (1984), 23B(3), 280-1 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

AB 1H NMR spectral data of compds. contg. 2,6-diphenylpiperidine moiety in the form of a monocyclic system or forming a part of fused bi-, tri- or tetracyclic ring structure show that the Ph groups attached to the carbon adjacent to the nitrogen, be it simple or simplex systems in which this moiety is embedded, exhibit the characteristic broad arom. proton signals with concurrent multiplicity due to nitrogen lone pair anisotropic effect.

IT 37123-09-4

RL: PRP (Properties)
(NMR of)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

13 ANSWER 63 OF 97 CAPLUS COPYRIGHT 2001 ACS

1984:423422 CAPLUS

DN 101:23422

TI Synthesis and transformations of polyhedral compounds. V. Synthesis and cyclization of some 3,7-diacyl-3,7-diazabicyclo[3.3.1]nonanes

AU Agadzhanyan, Ts. E.; Arutyunyan, G. L. CS Inst. Tonk. Org. Khim., Yerevan, USSR

SO Arm. Khim. Zh. (1983), 36(11), 730-4

CODEN: AYKZAN; ISSN: 0515-9628

DT Journal

LA Russian

GΙ

III

NCOR NCOR

Me

Ph

II

Me NCH₂Ph

IV

AB Ring cleavage of diazaadamantane I (R1 = Ph, X = O) by RCOCl (R = phthalimidomethyl, p-O2NC6H4, BrCH2) gave 46-56% diazabicyclononanes II. Similar ring cleavage of I (R1 = NO2, X = Me2) by Ac2O, TsCl, and RCOCl gave 15-67% of the corresponding II. Intramol. cyclization of III by PhCH2NH2 gave 51% IV.

IT 80808-87-3

RL: RCT (Reactant)

(intramol. cyclocondensation of, by benzylamine)

RN 80808-87-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(bromoacetyl)-1,5-dimethyl-(9CI) (CA INDEX NAME)

Page 190

The Marine F

ANSWER 64 OF 97 CAPLUS COPYRIGHT 2001 ACS

1984:191700 CAPLUS

100:191700

Synthesis and PMR spectral analysis of some N-chloropiperidin-4-ones and N-chloroazabicyclo[3.3.1]nonan-9-ones

ΑU Ganapathy, K.; Vijayan, B.

Dep. Chem., Annamalai Univ., Annamalainagar, 608 002, India CS

SO J. Indian Chem. Soc. (1983), 60(6), 572-4

CODEN: JICSAH; ISSN: 0019-4522

DΤ Journal

LΑ English

GΙ

R7 NCl $k^7 R^6$

ΙI

AB Chloropiperidinones I (R = H, Cl; R1 -R4 = H, Me Et, Me2CH, Bu, Ph) and chloroazabicyclo [3.3.1] nonan-9-ones II (X = CH2, CIN; R5 = H, Me, R6 = Ph, 2-ClC6H4, R7 = H, Ph) were prepd. and are good oxidizing agents. NMR spectra of I show a chair conformation. II except II (X = NCI, R5= H, R6 = R7 = Ph) have a twin-chair conformation; the exception has a chair-boat conformation. The equatorial H in I absorbs at higher field than the axial proton and the equatorial Me protons absorb at higher field than the axial Me protons. The equatorial Me group at C-3 or C-5 shields the vicinal axial H at C-2 or C-6 and the axial Me group at C-3 deshields the axial H at C-2. These effects were also seen in II.

IT 37123-09-4

RL: RCT (Reactant)

(chlorination of)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) INDEX NAME)

113 ANSWER 65 OF 97 CAPLUS COPYRIGHT 2001 ACS 1984:34525 CAPLUS

DN 100:34525

N-Chlorination and dehydrochlorination of aryl-substituted piperidines, 3-azabicyclo[3.3.1]nonanes, and 3,7-diazabicyclo[3.3.1]nonanes. Synthesis of the first 3,7-diazanoradamantane

AU Quast, Helmut; Mueller, Bodo

CS Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Fed. Rep. Ger.

SO Chem. Ber. (1983), 116(12), 3931-46

CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

GΙ

AB N-Chloropiperidine derivs. I and II (R = Cl, Rl = H, R2 = Ph, 4-ClC6H4, 4-MeC6H4; R3 = H, Ph, 4-MeC6H4; X = CH2, N+H2.Cl-, NCl) were obtained by chlorination using Me3COCl. Dehydrochlorination of I and II (R - R3 as above; X = CH2) gave I and II (RRl = bond). However, dehydrochlorination of II (R = Cl, Rl = H, R2 = R3 = 4-MeC6H4, X = NCl) gave 2,6-bis(4-methylphenyl)pyridine. Surprisingly, the spontaneous dehydrochlorination of chlorodiazabicyclo[3.3.1]nonane II (R = Cl, Rl = H, R2 = R3 = 4-MeC6H4, X = N+H2.Cl-) produced the highly strained 3,7-diazanoradamantane III (R4 = 4-MeC6H4). Its structure was assigned on the basis of high field 1H and 13C NMR spectra, nuclear Overhauser difference spectroscopy, and the temp. dependence of the 1H and 13C NMR spectra resulting from slow rotation of the 4-MeC6H4 groups. The barrier of rotation for the 1,3-diaxial oriented 4-MeC6H4 groups at C-6,8 was .DELTA.G247.thermod. = 50 .+-. 1 kJ.cntdot.mol-1.

IT 75549-49-4

RL: RCT (Reactant) (chlorination of)

RN 75549-49-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetrakis(4-methylphenyl)-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

ANSWER 66 OF 97 CAPLUS COPYRIGHT 2001 ACS

1983:612473 CAPLUS

DN 99:212473

TI Synthesis of spiro[2H-1,3-benzoxazine-2,4'-piperidines] from N,N'-dibenzylidenephenylmethanediamines and 2,6-diaryl-4-piperidones

AU Takajo, Tokiharu; Kambe, Satoshi

CS Coll. Technol., Oyama Natl. Coll. Technol., Oyama, 323, Japan

SO Synthesis (1983), (7), 564-6 CODEN: SYNTBF; ISSN: 0039-7881

DT Journal

LA English

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Spiro[benzoxazine-piperidines] I (R = H, Cl; Rl = H, Me) were obtained in 52-58% yield by treating [5,2-R(HO)C6H3CH:N]2CHC6H3(OH)R-2,5 (II) with piperidinones III (R2 = R3 = Me, R4 = H). Treatment of II with III (Rl = R2 = H, R3 = R4 = Ph) gave imines IV. Diazabicyclononanones V (Rl = Me, R5 = H; Rl = H, R5 = Me) were obtained by treating (4-R5C6H4CH:N)2CHC6H4R5-4 (VI) with III (Rl = H, Me, R2 = R3, H, R4 = Me). Pyridopyrimidines VII were obtained from VI and III (Rl = H, Me, R2 = R3 = Me, R4 = H).

IT 87731-90-6P

RN 87731-90-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4-bis(4-methylphenyl)-6,8-diphenyl- (9CI) (CA INDEX NAME)

Page 195

IX3

ANSWER 67 OF 97 CAPLUS COPYRIGHT 2001 ACS

1983:52782 CAPLUS

98:52782

TI Crystal and molecular structure of tetraaryl-3,7-diazabicyclo[3.3.1]nonanes and tetra- and pentaaryl-1,3-diazaadamantanes. Chair-boat conformation of the tetraaryl-3,7-diazabicyclo[3.3.1]nonanes

AU Quast, Helmut; Mueller, Bodo; Peters, Eva Maria; Peters, Karl; Von Schnering, Hans Georg

CS Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Fed. Rep. Ger.

SO Chem. Ber. (1982), 115(11), 3631-52 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Mannich reaction of 3,5-(Me3C)2C6H3CHO gave diarylpiperidinone I, while AB similar treatment of 3,5-Me2C6H3CHO gave diazabicyclononanone II (R = 3,5-xylyl, R1 = H) directly, along with diazaadamantanone III (R = 3,5-xylyl). Similarly, III (R = 4-tolyl) was isolated in the prepn. of II (R = 4-tolyl, R1 = H) (IV). Methylation of IV with MeI in refluxing Me2CO/C6H6 contq. K2CO3 gave II (R = 4-tolyl, R1 = Me); Wolff-Kishner redn. of IV gave V (R = 4-tolyl, R1 = H), which was monomethylated to give V (R = 4-tolyl, R1 = Me), regioselectively. X-ray anal. of II (R = 3,5-xylyl, R1 = H; R = 4-tolyl, R1 = Me), III, V (R = 4-tolyl, R1 = Me)and the diazaadamantanone VI gave the structures and preferred conformations, esp. those of the aryl groups, in the cryst. state. All tetraaryl-3,7-diazabicyclononanones exist in the chair-boat conformation with equatorial aryl groups. Two of the 5 aryl substituents in III occupy a 1,3-diaxial position, while the 3 neighboring aryl groups exhibit an unexpected propeller-like arrangement.

IT 83097-72-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and crystal and mol. structure of)

RN 83097-72-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(3,5-dimethylphenyl)-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

IT 75541-41-2P 83116-06-7P 84182-80-9P

RN 75541-41-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methylphenyl)-, hydrazone, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

RN 83116-06-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetrakis(3,5-dimethylphenyl)-, (1.alpha.,2.alpha.,4.alpha.,5.alpha.,6.beta.,8.beta.)- (9CI) (CA INDEX NAME)

RN 84182-80-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(3,5-dimethylphenyl)-,
hydrazone, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

09/623,726 ANSWER 68 OF 97 CAPLUS COPYRIGHT 2001 ACS 1983:16738 CAPLUS DN 98:16738 Bispidine derivatives and pharmaceutical compositions containing them ΤI Binnig, Fritz; Mueller, Claus D.; Raschack, Manfred; Von Philipsborn, ΙN Gerda BASF A.-G. , Fed. Rep. Ger. PA SO Ger. Offen., 9 pp. CODEN: GWXXBX DTPatent LA German FAN.CNT 1 APPLICATION NO. PATENT NO. KIND DATE DATE ΡI DE 3112055 A1 19821007 DE 1981-3112055 19810327 FI 8200529 A . 19820928 FI 1982-529 19820217 FI 71146 19860814 В FI 71146 С 19861124 IL 65163 IL 1982-65163 Α1 19840629 19820303 US 4459301 Α 19840710 US 1982-354515 19820303 NO 8200878 Α 19821004 NO 1982-878 19820317 JP 57165385 Α2 19821012 JP 1982-43012 19820319 JP 03043274 B4 19910701 EP 62199 **A1** EP 1982-102271 19821013 19820319 EP 62199 19840620 В1 R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE AT 8050 E 19840715 AT 1982-102271 19820319 DD 201795 Α5 19830810 DD 1982-238437 19820325 Α NO 8201018 19820928 NO 1982-1018 19820326 NO 157452 В 19871214 NO 157452 С 19880323 DK 1982-1389 DK 8201389 Α 19820928 19820326 DK 157813 В 19900219 DK 157813 С 19900716 AU 8281962 Α1 19820930 AU 1982-81962 19820326 AU 546256 В2 19850822 ES 510856 Α1 19830201 ES 1982-510856 19820326 HU 29934 0 19840228 HU 1982-945 19820326 HU 185516 В 19850228 FI 8201125 Α 19821003 FI 1982-1125 19820331 JP 57179044 A2 19821104 JP 1982-51464 19820331 DK 8201498 Α 19821003 DK 1982-1498 19820401 Α ZA 8202269 19830223 ZA 1982-2269 19820401 US 4556662 19851203 US 1983-537838 Α 19830930 PRAI DE 1981-3112055 19810327

19810402

19820303

19820319

$$R$$
—CON NCH₂Ph I

DE 1981-3113389

US 1982-354515

EP 1982-102271

AB Bispidines I (R = H, NH2) were prepd. Thus N-benzylbispidine was treated

Page 199

GI

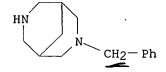
with 4-O2NC6H4COCl to give 82.5% I (R = NO2) which was hydrogenated on Pt-C to give 81% I (R = NH2).

IT 69407-32-5

RL: RCT (Reactant)
 (benzoylation of)

RN 69407-32-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



Page 200

ANSWER 69 OF 97 CAPLUS COPYRIGHT 2001 ACS

1982:615139 CAPLUS

N 97:215139

TI Conformational and configurational studies on 3-azabicyclo[3.3.1]nonane (3-ABN) derivatives and related systems employing carbon-13 NMR spectroscopy

AU Jeyaraman, R.; Jawaharsingh, Cooksley Baldwin; Avila, S.; Ganapathy, K.; Eliel, Ernest L.; Manoharan, Muthiah; Morris-Natschke, Susan

CS Dep. Chem., Am. Coll., Madurai, 625002, India

SO J. Heterocycl. Chem. (1982), 19(3), 449-58 CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

The 13C NMR of four cis-2,4-diphenyl-3-azabicyclo[3.3.1]nonanes, eleven cis-2,4-diaryl-3-azabicyclo[3.3.1]nonan-9-ones, twenty-six cis-2,4-diaryl-3-azabicyclo[3.3.1]nonan-9-ols or acetates, five cis-2,4-diaryl-3-azabicyclo[4.3.1]decan-10-ones or -10-ols and five cis-2,4-diphenyl-3-aza-7-thiabicyclo[3.3.1]nonan-9-ones, -9-ols of 9-yl acetates are obsd. Except for the 7-thia compds., which exist mainly in the configuration and conformation with the N atom-contg. ring in the boat form, these compds. exist overwhelmingly in chain-chair conformations. The configuration of the 9-ols and their acetates (syn or anti to the N-atom-contg. ring) is detd. from the spectra. In several cases, the structure assigned differ from those made earlier. Broadening of one set of aryl signals (probably those due to the o-C atoms) in the case of N-Me (but not N-H) compds. without ortho substituents is due to restricted Ph rotation.

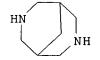
IT 280-74-0

RL: PRP (Properties)

(carbon-13 NMR of, conformation and configuration in relation to)

RN 280-74-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)



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09/,623,726
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ANSWI

ANSWER 70 OF 97 CAPLUS COPYRIGHT 2001 ACS

1982:562202 CAPLUS

DN 97:162202

TI Conformation in solution of tetraaryl-3,7-diazabicyclo[3.3.1]-nonanes and tetra- and pentaaryl-1,3-diazaadamantanes. A nuclear magnetic resonance study

AU Jackman, Lloyd M.; Dunne, Theresa S.; Mueller, Bodo; Quast, Helmut

CS Dep. Chem., Pennsylvania State Univ., University Park, PA, 16802, USA

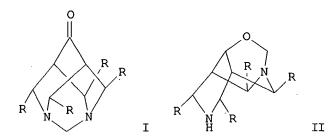
SO Chem. Ber. (1982), 115(8), 2872-91

CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA English

GΙ



The proton NMR spectra of a series of tetraaryl-3,7-AB diazabicyclo[3.3.1] nonanes, have been assigned with the aid of nuclear Overhauser difference spectroscopy. The NOE's together with spin lattice relaxation times show that these mols. adopt the chair-boat conformation with all aryl groups being equatorial. This conformation and the torsional angles of the aryl groups are similar to those found in the solid state. Analogous studies have been carried out with tetra- and pentaaryl-1,3-diazaadamantanes. A surprisingly low barrier of rotation (I; R = 3,5-Me2C6H3: .DELTA.G.+-.298 = 42 kJ.cntdot.mol-1) has been found for the two 1,3-diaxially oriented aryl groups in these systems; carbon-13 chem. shift data are reported for the above compds. Those of the 3,7-diazabicyclononanes are consistent with the proposed chair-boat conformation; nitrogen-15 chem. shift data and 13C-15N coupling consts. are also in accord with this conformation. A stereoselective redn. of I (R = 3, 5-Me2C6H3) to the corresponding alc. and the ready acid-catalyzed rearrangement of this alc. to II (R as above), the first example of the 9-oxa-1,5-diazatricyclo[5.3.1.33,8]undecane ring system, is described.

IT 75541-45-6 75549-49-4 75549-52-9

83097-72-7 83116-06-7

RL: PRP (Properties)

(conformation of, NMR in relation to)

RN 75541-45-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(4-methylphenyl)-6,8-diphenyl-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

RN 75549-49-4 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetrakis(4-methylphenyl)-,
(2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 75549-52-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methylphenyl)-, (2R,4S,6S,8R)-rel- (9CI) (CA INDEX NAME)

RN 83097-72-7 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(3,5-dimethylphenyl)-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 83116-06-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetrakis(3,5-dimethylphenyl)-,
(1.alpha.,2.alpha.,4.alpha.,5.alpha.,6.beta.,8.beta.)- (9CI) (CA INDEX NAME)

09/@23,726

ANSWER 71 OF 97 CAPLUS COPYRIGHT 2001 ACS 1982:406193 CAPLUS

DN 97:6193

Synthesis and pharmacological properties of 2,4,6,8-tetraphenylbispidin-9-ΤI

Ribalta, Miguel; Ribas, Jose Maria; Martinez Tobed, Antonio; Basi, Nuria; ΑU Zapatero, Jorge; Bruseghini, Leonida

Cent. Invest. Quim.-Farm., Invest. Tec. Apl. S.A., Barcelona, Spain CS

Eur. J. Med. Chem. - Chim. Ther. (1982), 17(2), 187-90 SO

CODEN: EJMCA5; ISSN: 0009-4374

DTJournal

LА English

GI

Bispidinones I (R = H, Me; R1 = H, 4-OMe, 2-Cl, 4-Cl; R2 = Et, Bu, CMe3, AB cyclohexyl, allyl, PhCH2; Z = O, S) were prepd. by N-carbamoylation; the compds. prepd. showed anticonvulsant, anticataleptic, myorelaxant, antidepressant, and antiulcer activity. 2,4,6,8-Tetraphenylbispidin-9-one was heated with BuNCO in CHCl3 to give I (R = R1 = H, Z = O, R2 = Bu).

IT 82058-25-1P 82058-26-2P 82058-27-3P

82058-28-4P 82058-29-5P 82058-30-8P

82058-31-9P 82058-32-0P 82058-33-1P

82058-34-2P 82058-35-3P 82058-36-4P

82058-37-5P 82058-38-6P 82058-39-7P

82058-40-0P 82058-41-1P 82058-42-2P

82058-43-3P 82058-44-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and pharmacol. activity of)

RN 82058-25-1 CAPLUS

3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-ethyl-9-oxo-2,4,6,8-CN tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-26-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-butyl-9-oxo-2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-27-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(1,1-dimethylethyl)-9-oxo-2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-28-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-cyclohexyl-9-oxo-2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-29-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-ethyl-1-methyl-9-oxo-2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-30-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-butyl-1-methyl-9-oxo-2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

RN . 82058-31-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-(1,1-dimethylethyl)-1-methyl-9-oxo-2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-32-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-cyclohexyl-1-methyl-9-oxo-2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-33-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, N-ethyl-9-oxo-2,4,6,8-

Page 208

tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-34-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, 9-oxo-2,4,6,8-tetraphenyl-N-2-propenyl-(9CI) (CA INDEX NAME)

RN 82058-35-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, 9-oxo-2,4,6,8-tetraphenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 82058-36-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, N-ethyl-1-methyl-9-oxo-2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

RN 82058-37-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, 1-methyl-9-oxo-2,4,6,8-tetraphenyl-N-2-propenyl- (9CI) (CA INDEX NAME)

Ph Me

$$Ph$$
 $C-NH-CH_2-CH=CH_2$
 Ph
 S

RN 82058-38-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, 1-methyl-9-oxo-2,4,6,8-tetraphenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 82058-39-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, N-ethyl-2,4,6,8-tetrakis(4-methoxyphenyl)-9-oxo-(9CI) (CA INDEX NAME)

RN 82058-40-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, N-ethyl-2,4,6,8-tetrakis(4-methoxyphenyl)-9-oxo- (9CI) (CA INDEX NAME)

Page 210

. Contraction of the Contraction

RN 82058-41-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 2,4,6,8-tetrakis(2-chlorophenyl)-N-ethyl-9-oxo- (9CI) (CA INDEX NAME)

RN 82058-42-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, 2,4,6,8-tetrakis(2-chlorophenyl)-N-ethyl-9-oxo- (9CI) (CA INDEX NAME)

RN 82058-43-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carboxamide, 2,4,6,8-tetrakis(4-chlorophenyl)-N-ethyl-9-oxo- (9CI) (CA INDEX NAME)

RN 82058-44-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3-carbothioamide, 2,4,6,8-tetrakis(4-chlorophenyl)-N-ethyl-9-oxo- (9CI) (CA INDEX NAME)

IT 55407-47-1 77737-97-4 82058-24-0

RL: RCT (Reactant)

(N-carbamoylation of, by Et isocyanate and isothiocyanate)

RN 55407-47-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methoxyphenyl)-(9CI) (CA INDEX NAME)

RN 77737-97-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-chlorophenyl)-(9CI) (CA INDEX NAME)

IT **37123-09-4 60823-94-1**RL: RCT (Reactant)

(N-carbamoylation of, by org. isocyanates and isothiocyanates)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 60823-94-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

ANSWER 72 OF 97 CAPLUS COPYRIGHT 2001 ACS

1982:104172 CAPLUS

DN 96:104172

TI Synthesis and reactions of polyhedral compounds. II. Synthesis of 5,7-dimethyl-1,3-diazaadamantan-6-one and -6-ol and their conversion into 3,7-diacyl(dicarbalkoxy, diarylsulfonyl)-3,7-diazabicyclo[3,3,1]nonanes

AU Agadzhanyan, Ts. E.; Arutyunyan, G. L.

CS Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR

SO Arm. Khim. Zh. (1981), 34(11), 963-8

CODEN: AYKZAN; ISSN: 0515-9628

DT Journal

LA Russian

GΙ

AB Cyclocondensation of EtCOEt, HCHO, and AcONH4 gave 19.5% I, which reacted with RCOCl, RO2CCl, or ArSO2Cl to give II [R = BrCH2CO, BrCH2CH2CO, CH2:CHCO, Bz, (phthalimidomethoxy)carbonyl, EtOCO, PhCH2OCO, 4-MeC6H4SO2, 4-(MeO2CNH)C6H4SO2]. LiAlH4 redn. of I gave 83.3% alc., which with ClCO2Et gave III.

IT 80808-87-3P 80808-88-4P 80808-89-5P 80808-91-9P 80808-92-0P 80808-93-1P

80808-96-4P 80808-99-7P

RN 80808-87-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(bromoacetyl)-1,5-dimethyl-(9CI) (CA INDEX NAME)

BrCH₂-C
$$\sim$$
 Me \sim C-CH₂Br \sim Me

RN 80808-88-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(3-bromo-1-oxopropyl)-1,5-dimethyl- (9CI) (CA INDEX NAME)

Page 216

in a substitution of the

$$\begin{array}{c|c} \text{BrCH}_2-\text{CH}_2-\text{C} \\ \text{N} \\ \text{N} \\ \text{Me} \end{array} \begin{array}{c} \text{C-CH}_2-\text{CH}_2\text{Br} \\ \text{Me} \\ \text{O} \end{array}$$

RN 80808-89-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3,7-bis(1-oxo-2-propenyl)-(9CI) (CA INDEX NAME)

RN 80808-91-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 1,5-dimethyl-9-oxo-, bis[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl] ester (9CI) (CA INDEX NAME)

RN 80808-92-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 1,5-dimethyl-9-oxo-, diethyl ester (9CI) (CA INDEX NAME)

RN 80808-93-1 CAPLUS

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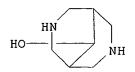
Lives Law Royalds

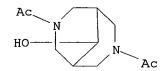
CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 1,5-dimethyl-9-oxo-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

RN 80808-96-4 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl- (9CI) (CA INDEX NAME)

RN 80808-99-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-3,7-dicarboxylic acid, 9-hydroxy-1,5dimethyl-, diethyl ester (9CI) (CA INDEX NAME)

09/623,726 ANSWER 73 OF 97 CAPLUS COPYRIGHT 2001 ACS 1981:497292 CAPLUS DN 95:97292 ΤI Synthesis of 6-O-benzoyl-1,3-diazaadamantane Aslanov, Kh. A.; Inoyatova, D. A.; Kosovskii, A. V.; Atabaev, R. ΑU USSR CS Sb. Nauch. Tr. Tashkent. Un-t (1979), (595), 83-6 SO From: Ref. Zh., Khim. 1981, Abstr. No. 7Zh217 DTJournal LА Russian Title only translated. AΒ IT 78693-65-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and benzoylation of) 78693-65-9 CAPLUS RN3,7-Diazabicyclo[3.3.1]nonan-9-ol (6CI, 9CI) (CA INDEX NAME) CN





ANSWER 74 OF 97 CAPLUS COPYRIGHT 2001 ACS

1981:425025 CAPLUS

DN 95:25025

TI Synthesis and reactions of ketones of 3-aza-, 3,7-diazabicyclononane and 3,7-diazaadamantane series

AU Omarov, T. T.; Baisalbaeva, S. A.; Gubasheva, A. Sh.

CS USSR

SO Tr. Inst. Khim. Nauk, Akad. Nauk Kaz. SSR (1980), 52, 147-70 CODEN: TIKNAG; ISSN: 0568-5087

DT Journal

LA Russian

GΙ

AB Condensation of cyclohexanone with BzH and H4NOAc gave a mixt. of diazabicyclononanone I and 2,6-dibenzylidenecyclohexanone. I was methylated. The diazabicyclononanes II (R = H, Me) were obtained by a similar condensation from the resp. piperidinone. The diazaadamantanes III were obtained from II by condensation with HCHO. III were reduced to alcs. I was converted to acetylenic alcs. Addnl. reactions of I, II and III were discussed. The conformation, spectra and biol. activity of I, II and III were discussed with 72 refs.

IT 37123-09-4P 60823-94-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and cyclocondensation of, with formaldehyde, diazaadamantane from)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 60823-94-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

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09/823.726
     ANSWER 75 OF 97 CAPLUS COPYRIGHT 2001 ACS
     1981:406994 CAPLUS
DN
     95:6994
     3,7-Diazabicyclo[3.3.1]nonan-9-ones, octahydropyrido[4,3-d]pyrimidines,
ΤI
     and 1,3,7-triazabicyclo[3.3.1]non-3-enes from N,N'-
     dibenzylidenephenylmethanediamines and alkyl methyl ketones
ΑU
     Takajo, Tokiharu; Kambe, Satoshi
     Oyama Tech. Coll., Tochigi, 323, Japan
CS
SO
     Synthesis (1981), (2), 151-3
     CODEN: SYNTBF; ISSN: 0039-7881
DT
     Journal
LA
     English
GI
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The cyclocondensation of RCH(N:CHR)2 (R = Ph, p-tolyl, 4-ClC6H4, 4-MeOC6H4) with MeCOCR1R2R3 [R1, R2, and R3 (same or different) are H or Me] gave the resp. diazabicyclononanones I, pyrido[4,3-b]pyrimidines II, and triazabicyclononenes III (from MeCOCMe3). A mixt. of PhCH(N:CHPh)2, MeCOEt, and NH4OAc in MeOH was stirred 2 days at room temp., kept 2 days, and worked up to give I (R = Ph, R1 = Me) and II (R = Ph, R1 = Me, R2 = H).

N 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 60823-94-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 77737-96-3 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 77737-97-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-chlorophenyl)-(9CI) (CA INDEX NAME)

RN 77841-40-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methylphenyl)-(9CI) (CA INDEX NAME)

ANSWER 76 OF 97 CAPLUS COPYRIGHT 2001 ACS 1981:156628 CAPLUS DN 94:156628 Chemistry of 3-azabicyclo[3.3.1] nonanes ΤI ΑU Jeyaraman, R.; Avila, S. CS Dep. Chem., American Coll., Madurai, 625002, India SO Chem. Rev. (1981), 81(2), 149-74 CODEN: CHREAY; ISSN: 0009-2665 DTJournal; General Review LΑ English A review with 339 refs. AΒ IT 280-74-0D, derivs. RL: MSC (Miscellaneous) (chem. of) RN280-74-0 CAPLUS 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME) CN



ANSWER 77 OF 97 CAPLUS COPYRIGHT 2001 ACS

1980:620339 CAPLUS

DN 93:220339

Stereochemistry of tetraaryl-3,7-diazabicyclo[3.3.1]nonanes and ΤI tetraaryl-1,3-diazaadamantanes

Quast, Helmut; Mueller, Bodo ΑU

Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Fed. Rep. Ger. CS

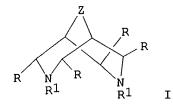
Chem. Ber. (1980), 113(9), 2959-75 SO

CODEN: CHBEAM; ISSN: 0009-2940

Journal DΤ

German LΑ

GΙ



2,4,6,8-Tetraaryl-3,7-diazabicyclo[3.3.1]nonanes I (Z = CH2, CO; R = Ph, AΒ p-tolyl; R1 = H) (II) were converted into the 1,3-diazaadamantanes (I; R12= CH2) (III) by reaction with paraformaldehyde; II have the rel-(2S,4R,6R,8S)- configuration and III have the rel-(4R,8S,9R,10S)configuration. The 1H NMR spectra show that II exist in the chair-chair conformation. The reaction of cis-2,6-diarylpiperidones with benzaldehydes yielded tetraaryldiazabicyclononanones in which the equatorial aryl groups of the piperidones prefer the axial positions in the diazabicyclononanones.

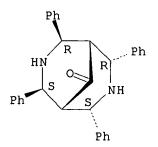
IT 65732-77-6P 75541-42-3P 75541-43-4P 75541-44-5P 75541-45-6P 75549-49-4P 75549-52-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction with paraformaldehyde)

RN 65732-77-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl-, (2R, 4S, 6S, 8R) - rel - (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 75541-42-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetraphenyl-, (2-endo,4-endo,6exo, 8-exo) - (9CI) (CA INDEX NAME)

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Relative stereochemistry.

RN 75541-43-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one-1,5-d2, 2,4,6,8-tetraphenyl-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 75541-44-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-diphenyl-6,8-di(phenyl-d5)-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

RN 75541-45-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(4-methylphenyl)-6,8-diphenyl-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 75549-49-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetrakis(4-methylphenyl)-, (2-endo,4-endo,6-exo,8-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 75549-52-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methylphenyl)-, (2R,4S,6S,8R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

75541-40-1P IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and redn. of)

75541-40-1 CAPLUS RN

3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl-, hydrazone, CN (2-endo, 4-endo, 6-exo, 8-exo) - (9CI) (CA INDEX NAME)

$$R \sim N-NH_2$$

IT 75541-41-2P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 75541-41-2 CAPLUS

RN

3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methylphenyl)-, CN hydrazone, (2-endo, 4-endo, 6-exo, 8-exo) - (9CI) (CA INDEX NAME)

IT 75598-03-7

RL: RCT (Reactant)

(reaction of, with paraformaldehyde)

RN 75598-03-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 2,4,6,8-tetraphenyl- (9CI) (CA INDEX NAME)

L13 ANSWER 78 OF 97 CAPLUS COPYRIGHT 2001 ACS
AN 1979:501880 CAPLUS
DN 91:101880
TI Antiarrhythmic activity of some N-alkylbispidinebenzamides
AU Ruenitz, Peter C.; Mokler, Corwin M.
CS Sch. Pharm., Univ. Georgia, Athens, GA, 30602, USA
J. Med. Chem. (1979), 22(9), 1142-4
CODEN: JMCMAR; ISSN: 0022-2623
DT. Journal
LA English
GI

 R^1 n CON NR @X

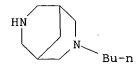
Nine bispidinebenzamides I (R = Me or Bu; R1 = H, OMe, or C1; n = 1, 2, or 3; X = HCl or fumarate) were synthesized by condensation of N-methyl-[58324-99-5] or N-butylbispidine [58325-01-2] with the appropriate acid chlorides. The synthesized compds. were evaluated in mice for acute toxicity and their ability to protect against chloroform-induced ventricular fibrillation. All of them were active. I; R = Me, R1 = H, X = fumarate [70802-37-8], I; R = Me, R1 = 4-MeO, X = fumarate [70802-39-0], and I; R = Me, R1 = 4-C1, X = fumarate [71004-34-7] had potencies and LD50-to-ED50 ratios comparable to those of disopyramide. However, their potencies in increasing the effective refractory period in isolated rabbit atria were considerably less than that of disapyramide.

IT 58325-01-2

RL: BIOL (Biological study)
(condensation of, with Ph acid chlorides)

RN 58325-01-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl- (9CI) (CA INDEX NAME)



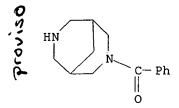
IT 70802-35-6DP, derivs.

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and antiarrhythmic activity of)

RN 70802-35-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-benzoyl- (9CI) (CA INDEX NAME)



ANSWER 79 OF 97 CAPLUS COPYRIGHT 2001 ACS

🗚 🥄 1979:121568 CAPLUS

DN 90:121568

TI Bispidine derivatives

IN Binnig, Fritz; Friedrich, Ludwig; Hofmann, Hans Peter; Kreiskott, Horst; Raschack, Manfred; Mueller, Claus

PA BASF A.-G., Ger.

SO Ger. Offen., 14 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

FAN.	CNT 1 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 2726571	A1	19781221	DE 1977-2726571	19770613
	JP 54012398	A2	19790130	JP 1978-68375	19780608
	FI 7801872	Α	19781214	FI 1978-1872	19780612
	FI 63403	В	19830228		
	FI 63403	С	19830610		
	AT 7804265	Α	19810215	AT 1978-4265	19780612
	AT 363937	В	19810910		
	EP 74	A1	19781220	EP 1978-100147	19780613
	EP 74	B1	19800806		
	R: BE, CH,	DE, FR	, GB, NL, SE		
	US 4183935	Α	19800115	US 1978-915119	19780613
	CA 1105023	A1	19810714	CA 1978-305369	19780613
	AT 8003551	Α	19810215	AT 1980-3551	19800708
	AT 363938	В	19810910		
PRAI	DE 1977-2726571		19770613		
	AT 1978-4265		19780612		
GI			•		

$$R^{1}$$
 $CHR^{5}N$ $NCHR^{6}$ R^{4} I

The bispidine derivs. I (R1-R4 = H, F, Cl, alkyl, alkoxy, F3C, NO2; R5, R6 = H, Ph) and their salts were prepd. Thus, N,N'-dibenzylbispidine was hydrogenated (Pd/C) to give monobenzylbispidine, which was treated with 3-ClC6H4CH2Cl to give I (R1 = Cl, R2-R6 = H). At 1-20 mg/kg I were antiarrhythmic, calcium antagonists, antiphlogistic, and antithrombic.

IT 69407-32-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and benzylation of)

RN 69407-32-5 CAPLUS

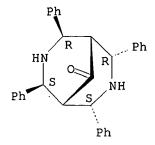
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)

ordusa

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09/6/23.726
     ANSWER 80 OF 97 CAPLUS COPYRIGHT 2001 ACS
     1978:104541 CAPLUS
DN
     88:104541
     Conformational studies on bicyclic compounds containing hetero atoms:
ΤI
     Part I. Synthesis and stereochemistry of some substituted
     azabicyclo[3.3.1]nonan-9-ones and azabicyclo[3.3.1]nonan-9-ols
     Baliah, V.; Usha, R.
ΑU
     Dep. Chem., Annamalai Univ., Annamalainagar, India
CS
     Indian J. Chem., Sect. B (1977), 15(8), 684-9
SO
     CODEN: IJSBDB
DT
     Journal
LΑ
     English
     Substituted 3-aza-, 3,7-diaza- and 3-thia-7-azabicyclo[3.3.1]nonan-9-ones
AΒ
     subjected to Meerwein-Ponndorf-Verley (MPV) and LiAlH4 redns. gave 2
     isomeric azabicyclo[3.3.1]nonan-9-ols (.beta.- and .alpha.-forms). The
     stereochem. course of the redn. is discussed.
IT
     65712-24-5
     RL: PRP (Properties)
        (IR spectrum of, conformation in relation to)
RN
     65712-24-5 CAPLUS
CN
     3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-2,4,6,8-tetraphenyl-,
     (2-endo, 4-endo, 6-exo, 8-exo) - (9CI) (CA INDEX NAME)
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Relative stereochemistry.

RN 65732-77-6 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl-, (2R,4S,6S,8R)-rel- (9CI) (CA INDEX NAME) Relative stereochemistry.



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09/623,726
     ANSWER 81 OF 97 CAPLUS COPYRIGHT 2001 ACS
     1977:601848 CAPLUS
DN
     87:201848
     Cytisine oxidation products (new synthesis of 1,3-diazaadamantane)
TI
     Orazgel'dyev, K. O.; Aslanov, Kh. A.; Sadykov, A. S.
ΑU
CS
     USSR
SO
     Sb. Nauch. Rabot. Turkm. NII Selektsii i Semenovodstva Tonkovoloknist.
     Khlopchatnika (1976), (14), 156-68
     From: Ref. Zh., Khim. 1977, Abstr. No. 4E102
DT
     Journal
     Russian
LΑ
     Title only translated.
AΒ
ΙT
     280-74-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and cyclocondensation reactions of)
     280-74-0 CAPLUS
RN
```

3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)



CN



CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

64974-38-5 CAPLUS RN

3,7-Diazabicyclo[3.3.1]nonane, compd. with 2,4,6-trinitrophenol (1:2) CN

(9CI) (CA INDEX NAME)

CM 1

CRN 280-74-0

CMF C7 H14 N2

HN

CM 2

CRN 88-89-1

CMF C6 H3 N3 O7

64974-39-6 CAPLUS RN

3,7-Diazabicyclo[3.3.1] nonane, compd. with 2,4-dihydro-5-methyl-4-nitro-2-CN

(4-nitrophenyl)-3H-pyrazol-3-one (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 550-74-3

C10 H8 N4 O5 CMF

$$\begin{array}{c|c} \text{Me} & \text{N} & \\ \hline & \text{N} & \\ \hline & \text{NO}_2 & \\ \end{array}$$

2 CM

280-74-0 CRN

CMF C7 H14 N2



ANSWER 82 OF 97 CAPLUS COPYRIGHT 2001 ACS 1977:29974 CAPLUS 86:29974 DN Use of the Mannich reaction in the synthesis of bispidine ΤI Ruenitz, Peter C.; Smissman, Edward E. ΑU CS Sch. Pharm., Univ. Kansas, Lawrence, Kans., USA SO J. Heterocycl. Chem. (1976), 13(5), 1111-13 CODEN: JHTCAD DTJournal English LΑ GΙ

RN $Z \rightarrow NR$ II, R=CH₂Ph, Z=H₂ III, R=H, Z=H₂

AB N,N'-dibenzylbispidinone (I), obtained by Mannich condensation of
N-benzyl-4-piperidone, was reduced (modified Wolff-Kishner) to give
N,N'-dibenzylbispidine (II), whose hydrogenolysis gave bispidine (III).
IT 280-74-0P
RL: PREP (Preparation)
 (by Mannich reaction of benzylpiperidine with benzylamine and formaldehyde)
RN 280-74-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME)



09/\$23,726

A ANSWER 83 OF 97 CAPLUS COPYRIGHT 2001 ACS

N 1976:577361 CAPLUS

DN 85:177361

TI Synthesis and stereochemistry of bicyclononane and adamantane heteroanalogs. III. Synthesis and some reactions of diazaadamantanes AU Azerbaev, I. N.; Omarov, T. T.; Baisalbaeva, S. A.; Bazalitskaya, V. S.

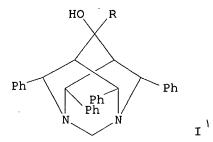
CS Inst. Khim. Nauk, Alma-Ata, USSR

SO Izv. Akad. Nauk Kaz. SSR, Ser. Khim. (1976), 26(4), 55-7 CODEN: IKAKAK

DT Journal

LA Russian

GI



AB Diazabicyclononane I (R = C.tplbond.CH), obtained in 83.4% yield by addn. of HC.tplbond.CH to the corresponding ketone, was hydrogenated to give 94.4% I (R = Et) and treated with amines and CH2O in a Mannich reaction to give satisfactory yields of I (R = Et2NCH2, piperidinomethyl).

IT 37123-09-4 60823-94-1

RL: RCT (Reactant)

(cyclocondensation of, by formaldehyde)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 60823-94-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

2.10分布整金线20·1

09/628,726

AS ANSWER 84 OF 97 CAPLUS COPYRIGHT 2001 ACS

N 1976:560045 CAPLUS

DN 85:160045

TI Nitrogen compounds of adamontane. IX. Preparation and reactions of nitrogen analogs of adamantane

AU Kafka, Zdenek; Galik, Vlastimil; Safar, Milan

CS Lab. Synth. Fuels, Prague Inst. Chem. Technol., Prague, Czech.

SO Sb. Vys. Sk. Chem.-Technol. Praze, Technol. Paliv (1976), D32, 127-57 CODEN: SVCTA6

DT Journal

LA Czech

Substituted 1-aza-, 1,3-diaza-, 1,3,5-triazaadamantanes (I), and AΒ 1,3-diazaadamantan-6-ols (II) and their derivs. were prepd. and characterized by ir, gas chromatog., and paper chromatog. Reaction of Me2CO, AcONH4, and arom. aldehydes gave tetrasubstituted 3,7-diazabicyclo[3.3.1]nonan-9-ones, which gave 1,3-diazaadamantan-6-ones on boiling with paraformaldehyde. These compds. were hydrogenated to tetracyclohexyl derivs. of II over Raney Ni. The 7-nitro deriv. of I was prepd. and reduced to the 7-amino deriv. with Zn or Al in alk. medium. The latter compd. gave 7-halo compds. and other derivs. Arom. aldehydes and the 7-amino deriv. of I gave aldimines, which were hydrogenated to secondary amines. I was stable in mineral acids but not in a reducing acid medium. Reductive methylation of the 7-amino deriv. of I gave 7-alkylamino deriv. The nitrile of N-(1,3,5-triaza-1adamantyl)aminoacetic acid, prepd. by cyanomethylation, was reduced to the 7-(aminomethyl)amino deriv. with LiAlH4. Partial hydrogenation of the 7-nitro deriv. of I gave the 7-hydroxylamino deriv., which with hexamethyldisilazane gave the trimethylsilyl deriv. Oxidn. with H2O2 or ozonization of the 7-nitro deriv. of I gave the N-oxide.

IT 37123-09-4P 55407-49-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and hydrogenation of)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 55407-49-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetra-3-pyridinyl- (9CI) (CA INDEX NAME)

IT 55407-47-1P 55407-51-7P 55407-53-9P

RN 55407-47-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methoxyphenyl)-(9CI) (CA INDEX NAME)

RN 55407-51-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 2,4,6,8-tetracyclohexyl- (9CI) (CA INDEX NAME)

RN 55407-53-9 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 2,4,6,8-tetra-3-pyridinyl- (9CI) (CA INDEX NAME)

ANSWER 85 OF 97 CAPLUS COPYRIGHT 2001 ACS

1976:542478 CAPLUS

DN 85:142478

TI Stereoisomerism of nitrogen p-electrons in some derivatives of azabicyclononane and azaadamantane

AU Azerbaev, I. N.; Omarov, T. T.; Al'mukhanova, K.; Baisalbaeva, S. A.

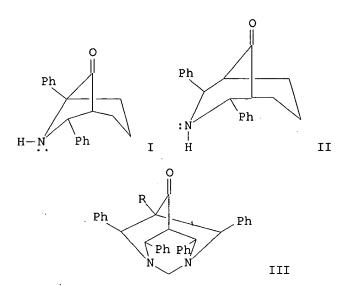
CS USSR

SO Zh. Org. Khim. (1976), 12(6), 1207-9 CODEN: ZORKAE

DT Journal

LA Russian

GΙ



AB Isomeric I and II were isolated and characterized by their ir spectra. Their configurational assignments were supported by cyclization of the corresponding diazabicyclononanes to give III (R = H, Me).

IT 55588-88-0 55648-00-5

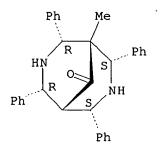
RL: RCT (Reactant)

(cyclization of, with formaldehyde)

RN 55588-88-0 CAPLUS

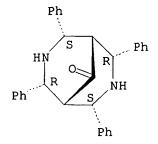
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl-, (endo,endo,endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 55648-00-5 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl-, (endo,endo,endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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09/623,726
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ANSWER 86 OF 97 CAPLUS COPYRIGHT 2001 ACS

1976:180182 CAPLUS AAÑ

DN 84:180182

Analogues of sparteine. II. Synthesis of N-monoalkylbispidines and ΤI N, N'-dialkylbispidines

Smissman, Edward E.; Ruenitz, Peter C. ΑU

Sch. Pharm., Univ. Kansas, Lawrence, Kans., USA CS

J. Org. Chem. (1976), 41(9), 1593-7 SO CODEN: JOCEAH

DT Journal

English LΑ

GΙ For diagram(s), see printed CA Issue.

Bispidines I, structurally related to antiarrhythmic oxytocic sparteine, AΒ were prepd. The condensation of piperidones II (R = Me, Bu) with PhCH2NH2 and CH2O, followed by a modified Wolff-Kishner redn. gave I (R = Me, Bu; R1 = PhCH2). Hydrogenolysis of I (R1 = PhCH2) gave the N-alkylbispidines I (R = Me, Bu; R1 = H), which were acylated and then reduced using LiAlH4 to N,N'-dialkylbispidines I (R = Me, Bu; R1 = Et, PhCH2). Alkylation of I (R = Me, Bu, R1 = H) gave I (R = Me, R1 = Et, Bu, cyclohexylmethyl; R = R1 = Bu).

IT 58375-24-9P

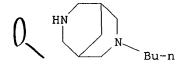
> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

58375-24-9 CAPLUS RN

3,7-Diazabicyclo[3.3.1]nonane, 3-butyl-, compd. with 2,4,6-trinitrophenol CN (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 58325-01-2 CMF C11 H22 N2



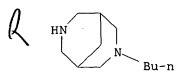
2 CM

CRN 88-89-1 CMF C6 H3 N3 O7

IT 58325-01-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn., alkylation, and acylation of)

RN58325-01-2 CAPLUS CN 3,7-Diazabicyclo[3.3.1]nonane, 3-butyl- (9CI) (CA INDEX NAME)



L13 ANSWER 87 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1975:578789 CAPLUS

DN 83:178789

TI Synthesis of 3-aza-3-methylbicyclo[3.3.1]nonan-9-one and some derivatives

AU Azerbaev, I. N.; Omarov, T. T.; Gubasheva, A. Sh.

CS USSR

SO Dokl. Resp. Nauchno-Tekh. Konf. Neftekhim., 3rd (1974), Volume 1, 437-9. Editor(s): Sarbaev, T. G. Publisher: Akad. Nauk Kaz. SSR, Inst. Khim. Nefti Prir. Solei, Guryev, USSR.

CODEN: 31GMAE

DT Conference

LA Russian

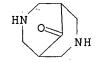
AB 2,4-Diphenyl-3-methyl-3-azabicyclo[3.3.1]nonan-9-one (I), bicyclo[3.3.1]nonan-9-one, and 3-aza-7-oxabicyclo[3.3.1]nonan-9-one were prepd. In the azabicyclononanones the unpaired electron pair on N influenced the reactivity of the ketones due to the interaction between the C:O group and the increased electron d. on the N; their C=O groups were less reactive than the C:O groups in other heterocyclic ketones. E.g., I was thoroughly hydrogenated on Pt oxide; on Raney Ni no H was absorbed. Very small yields were obtained from condensation reactions of the ketones. Alcs. were prepd. from the resp. ketones by treatment with Na in alc., Grignard reagents, C2H2 in the presence of alkali.

IT 57155-41-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reactivity of)

RN 57155-41-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one (9CI) (CA INDEX NAME)



ANSWER 88 OF 97 CAPLUS COPYRIGHT 2001 ACS 1975:514343 CAPLUS DN 83:114343

TI Synthesis of 2,4-diphenyl-6,6,8,8-tetramethyl-3,7-diazaadamanthan-10-one AU Azerbaev, I. N.; Omarov, T. T.; Baisalbaeva, S. A.

CS Inst. Khim. Nauk, Alma-Ata, USSR

SO Zh. Obshch. Khim. (1975), 45(6), 1404 CODEN: ZOKHA4

DT Journal

LA Russian

GI For diagram(s), see printed CA Issue.

AB The title compd. I was prepd. in 82% yield by cyclization of 2,4-diphenyl-6,6,8,8-tetramethyl-3,7-diazabicyclo[3.3.1]nonan-10-one with HCHO.

IT 56733-16-5

RL: RCT (Reactant)

(cyclization reaction with formaldehyde)

RN 56733-16-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,2,4,4-tetramethyl-6,8-diphenyl-(9CI) (CA:INDEX NAME)

3 ANSWER 89 OF 97 CAPLUS COPYRIGHT 2001 ACS

AN 1975:170823 CAPLUS

DN 82:170823

TI Nitrogen compounds of adamantae. V. Reaction of tetrasubstituted bispidones and 1,3-diazaadamanthanones

AU Kafka, Z.; Galik, V.; Safar, M.

CS Lab. Synth. Fuels, Inst. Chem. Technol., Prague, Czech.

SO Collect. Czech. Chem. Commun. (1975), 40(1), 174-8 CODEN: CCCCAK

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB Hydrogenation of the diazabicyclononane I and diazaadamantanones II (X = O, R = Ph, 4-MeOC6H4, 3-pyridyl) on Raney Ni at 150-200.degree. and 100 atm gave I and II (X = H, OH; R = cyclohexyl, 4-methoxycyclohexyl, 3-pyridyl). Hydrogenation of II (X = O, R = 3-pyridyl) also gave 23% 2,6-di(3-pyridyl)piperidin-4-ol.

IT 37123-09-4P 55407-47-1P 55407-49-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and hydrogenation of)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 55407-47-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetrakis(4-methoxyphenyl)-(9CI) (CA INDEX NAME)

RN 55407-49-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetra-3-pyridinyl- (9CI) (CA INDEX NAME)

IT 55407-51-7P 55407-53-9P

RN 55407-51-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 2,4,6,8-tetracyclohexyl- (9CI) (CA INDEX NAME)

RN 55407-53-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 2,4,6,8-tetra-3-pyridinyl- (9CI) (CA INDEX NAME)

A ANSW

ANSWER 90 OF 97 CAPLUS COPYRIGHT 2001 ACS

1975:156245 CAPLUS

DN 82:156245

TI Synthesis and stereochemistry of bicyclononane hetero analogs. II. Synthesis of some aza- and diazabicyclo[3.3.1]nonan-9-ones

AU Azerbaev, I. N.; Omarov, T. T.; Gubasheva, A. Sh.; Al'mukhanova, K. A.; Baisalbaeva, S. A.

CS USSR

SO Vestn. Akad. Nauk Kaz. SSR (1975), (2), 47-50 CODEN: VANKAM

DT Journal

LA Russian

GI For diagram(s), see printed CA Issue.

AB Mannich reaction of cyclohexanone, PhCHO, and NH4OAc gave 54% 2,4-diphenyl-3-azabicyclo[3.3.1]nonan-9-one and 31% 2,6-diphenylidenecyclohexanone. Similar reaction of 2,6-diphenyl-N-piperidinone (I) and 3-methyl-2,6-diphenyl-4-piperidinone (II) gave the diazabicyclononanones III (R = H, Me) via stereospecific condensation at the axial protons at C-3 and C-5 of I and II. The rate of condensation of II was less than that of I and 3,5-dimethyl-2,6-diphenyl-4-piperidinone did not react at all.

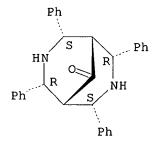
IT 55588-87-9P 55588-88-0P 55588-89-1P

55648-00-5P

RN 55588-87-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl-, dihydrochloride, (endo,endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

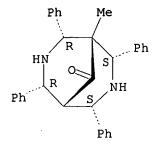


°●2 HCl

RN 55588-88-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-2,4,6,8-tetraphenyl-, (endo,endo,endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



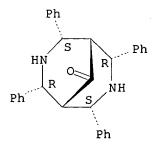
RN 55588-89-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 5-methyl-2,4,6,8-tetraphenyl-, dihydrochloride, (endo,endo,endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HC1

Relative stereochemistry.



ANSWER 91 OF 97 CAPLUS COPYRIGHT 2001 ACS

► 1975:80110 CAPLUS

DN 82:80110

TI Nitrogen compounds of adamantane. IV. Paper chromatography of azaadamantane derivatives

AU Kafka, Z.; Safar, M.; Galik, V.

CS Lab. Synth. Fuels, Inst. Chem. Technol., Prague, Czech.

SO Collect. Czech. Chem. Commun. (1974), 39(11), 3268-71

CODEN: CCCCAK

DT Journal

LA English

AΒ The sepn. of 1-azaadamantane (I) and its quaternary salts, 1,3-diazaadamantane (II) and its tetrasubstituted derivs., and 1,3,5-triazaadamantane (III) and its derivs. was studied by descending chromatog. on Whatman no. 1 paper at 20.degree.. The Rf values in various solvents are tabulated. Good sepn. of I and its quaternary salts was achieved by using a solvent system contg. HCl and an alc. with a branched chain, e.g. iso-PrOH or 2-methyl-1-propanol. For the sepn. of II and its derivs., HCl was replaced by HOAc; but the best results were obtained by using 20:1:4 EtOH-NH4OH(25%)-H2O. For the sepn. of III and its derivs. a neutral solvent system, i.e. alcs.-H2O was used. For the detection of I and II and their derivs., Dragendorff's reagent was used. To detect III and its derivs., which do not contain either a primary or a secondary amino group, a soln. of 4-dimethylaminobenzaldehyde in EtOH and HCl was used. The quaternary salts of I and derivs. of III were applied as aq. solns.; derivs. of II were dissolved in HOAc or in EtOH-HCl.

IT 55407-49-3 55407-53-9

RL: ANST (Analytical study); PROC (Process)
 (sepn. of, by paper chromatog.)

RN 55407-49-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetra-3-pyridinyl- (9CI) (CA INDEX NAME)

RN 55407-53-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 2,4,6,8-tetra-3-pyridinyl- (9CI) (CAINDEX NAME)

ANSWER 92 OF 97 CAPLUS COPYRIGHT 2001 ACS 1973:442379 CAPLUS 79:42379 TΙ Nitrogen-containing adamantanoid compounds. II. Synthesis of 1,3-diazoadamantane ΑU Galik, Vlastimil; Landa, Stanislav Vys. Sk. Chem. Technol., Prague, Czech. CS SO Collect. Czech. Chem. Commun. (1973), 38(4), 1101-3 CODEN: CCCCAK DTJournal LА German GΙ For diagram(s), see printed CA Issue. 1,3-Diazaadamantane (I) was prepd. CH2[CH(CO2Et)2]2 via CH2-[CH(CH2OH)2]2, CH2[CH(CH2Br)2]2, and 3,7-diazabicyclo- [3.3.1]nonane (II). II refluxed in C6H6 with paraformaldehyde gave I. ΙT 280-74-0 RL: RCT (Reactant) (reaction of, with paraformaldehyde, diazaadamantane by) RN280-74-0 CAPLUS 3,7-Diazabicyclo[3.3.1]nonane (6CI, 8CI, 9CI) (CA INDEX NAME) CN



ANSWER 93 OF 97 CAPLUS COPYRIGHT 2001 ACS

AM 1972:501556 CAPLUS

DN 77:101556

TI Synthesis of 3-thia-7-aza- and 3,7-diazabicyclo[3.3.1] nonane derivatives

AU Baliah, V.; Usha, R.

CS Dep. Chem., Annamalai Univ., Annamalainagar, India

SO Indian J. Chem. (1972), 10(3), 319-20

CODEN: IJOCAP

DT Journal

LA English

IT

GI For diagram(s), see printed CA Issue.

AB 2,4-Diphenyl-6,8-diaryl-3-thia-7-azabicyclo[3.3.1]nonan-9-ones e.g. I were prepd. by condensing both cis- and trans-2,6-diphenyltetrahydrothiapyran-4-one with aromatic aldehydes and ammonium acetate in EtOH. A similar condensation using 2,6-diphenyl-4-piperidone gives 2,4-diphenyl-6,8-diaryl-3,7-diazabicyclo[3.3.1]nonan-9-ones e.g. II.

37123-09-4P 37123-10-7P 37123-11-8P

37123-12-9P 37123-13-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 37123-09-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4,6,8-tetraphenyl- (6CI, 9CI) (CA INDEX NAME)

RN 37123-10-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(4-chlorophenyl)-6,8-diphenyl-(9CI) (CA INDEX NAME)

RN 37123-11-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(2-chlorophenyl)-6,8-diphenyl-(9CI) (CA INDEX NAME)

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RN 37123-12-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(4-methoxyphenyl)-6,8-diphenyl-(9CI) (CA INDEX NAME)

RN 37123-13-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2,4-bis(1,3-benzodioxol-5-yl)-6,8-diphenyl- (9CI) (CA INDEX NAME)

ANSWER 94 OF 97 CAPLUS COPYRIGHT 2001 ACS

1972:71608 CAPLUS

DN 76:71608

TI NMR spectra of substituted 3,7-diazabicyclo[3.3.1]nonan-9-ones

AU Haller, R.; Unholzer, H.

CS Pharm. Inst., Univ. Freiburg, Freiburg/Br., Ger.

SO Arch. Pharm. (Weinheim) (1971), 304(11), 866-71 CODEN: APBDAJ

DT Journal

LA German

GI For diagram(s), see printed CA Issue.

AB The 60- and 220-MHz PMR spectra of the title compds. (I, R = 2-pyridyl, 3-pyridyl, 4-pyridyl, or 6-methyl-2-pyridyl; R1 = Me or Et; R2 = Me or CH2Ph) and some of their N3-d derivs. in CDCl3 were examd. and the coupling consts. and chem. shifts vs. Me4Si as internal std. were detd. Couplings between vicinal NH and CH protons were obsd. in (3-pyridyl)-substituted I. The NMR spectra in relation to the configuration of I were discussed.

IT 5184-93-0 5498-19-1 35569-34-7 35569-36-9 35569-38-1 35612-71-6 RL: PRP (Properties)

: PRP (Properties (NMR of)

RN 5184-93-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-7- (phenylmethyl)-2,4-di-2-pyridinyl-, dimethyl ester (9CI) (CA INDEX NAME)

RN 5498-19-1 CAPLUS

CN 3,4-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-7- (phenylmethyl)-2,4-di-3-pyridinyl-, diethyl ester (9CI) (CA INDEX NAME)

RN 35569-34-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(3-methyl-2-pyridinyl)-9-oxo-7-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

RN 35569-36-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-7-(phenylmethyl)-2,4-di-3-pyridinyl-, dimethyl ester (9CI) (CA INDEX NAME)

RN 35569-38-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-7-(phenylmethyl)-2,4-di-4-pyridinyl-, diethyl ester (9CI) (CA INDEX NAME)

RN 35612-71-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,4-dicarboxylic acid, 9-oxo-3(phenylmethyl)-6,8-di-2-pyridinyl-, diethyl ester (9CI) (CA INDEX NAME)

ANSWER 95 OF 97 CAPLUS COPYRIGHT 2001 ACS

N 1972:3821 CAPLUS

DN 76:3821

TI Substituted 3,7-diazabicyclo[3.3.1]nonan-9-ols

AU Haller, R.; Unholzer, H.

CS Pharm. Inst., Univ. Freiburg, Freiburg/Breisgau, Ger.

SO Arch. Pharm. (Weinheim) (1971), 304(9), 654-9

CODEN: APBDAJ

DT Journal LA German

GI For diagram(s), see printed CA Issue.

AB The title compds. (I, R = H or Me, R1 = 2- or 3-pyridyl, R2 = Me or Et, R3 = Me or CH2Ph) were prepd. by redn. of the corresponding 9-oxo compds. with NaBH4 at very high stereoselectivity. The stereochemistry of the metholodide of I (R = H, R1 = 2-pyridyl, R2 = R3 = Me) was elucidated by nuclear Overhauser effect measurements.

IT 36332-85-1P

RN 36332-85-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-hydroxy-7-(phenylmethyl)-2,4-di-2-pyridinyl-, dimethyl ester, (endo,endo,syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 96 OF 97 CAPLUS COPYRIGHT 2001 ACS

1969:101290 CAPLUS

DN 70:101290

TI Metal chelates of (2-pyridyl)-substituted 3,7-diazabicyclo[3.3.1]nonanones

AU Haller, Rolf

CS Pharm. Inst., Univ. Freiburg/Br., Freiburg/Br., Ger.

SO Arch. Pharm. (Weinheim) (1969), 302(2), 113-18

CODEN: APBDAJ

DT Journal

LA German

GI For diagram(s), see printed CA Issue.

AB Hot alc. L reacts with an equal molar quant. of alc. transition metal salt to give MEX2 (M, X, R, R1, yield (%), m.p. (decompn.) given): Fe, SCN, Me, CH2Ph, 89, -; Co, SCN, Me, CH2Ph, 74, 210-12.degree.; Cd, SCN, Me, CH2Ph, 69, 180.degree.; Ni, SCN, Et, CH2Ph, 76, 212-15.degree.; Mn, Cl, Et, Me, 71, 242.degree. The ir spectra studied indicate that the azabicyclic complexes contain tetradentate ligands.

IT 4698-62-8 5184-93-0

RL: PRP (Properties) (spectrum of, ir)

RN 4698-62-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-benzyl-9-oxo-2,4-di-2-pyridyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)

5184-93-0 CAPLUS

.CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-7- (phenylmethyl)-2,4-di-2-pyridinyl-, dimethyl ester (9CI) (CA INDEX NAME)

RN

09/623,726 ANSWER 97 OF 97 CAPLUS COPYRIGHT 2001 ACS 1968:436077 CAPLUS DN 69:36077 A novel ring closure and amine quaternization under Eschweiler-Clarke ΤI conditions ΑU Smissman, Edward E.; Weis, James A. Sch. of Pharm., Univ. of Kansas, Lawrence, Kans., USA CS J. Heterocycl. Chem. (1968), 5(3), 405 SO CODEN: JHTCAD DTJournal English LА GΙ For diagram(s), see printed CA Issue. AΒ

1,3-Diazaadamantane sulfate (I) is prepd. 3,7-Diazabicyclo[3.3.1]nonane sulfate (II) is treated with HCHO and HCO2H to give 1,3-diazaadamantane-1methonium sulfate (III). N.M.R. data for I and III are given.

ΙT 20027-05-8 RL: RCT (Reactant) (cyclization of) 20027-05-8 CAPLUS RN

CN3,7-Diazabicyclo[3.3.1]nonane, sulfate (1:1) (8CI) (CA INDEX NAME)

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CM 7664-93-9 CRN CMF H2 O4 S

CM

CRN 280-74-0 C7 H14 N2 CMF

